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► To cite this version:

Marianne Bessemoulin-Chatard, Mazen Saad. Preserving monotony of combined edge finite volume–finite element scheme for a bone healing model on general mesh. *Journal of Computational and Applied Mathematics*, 2017, 309, pp.287-311. 10.1016/j.cam.2016.07.004 . hal-01153975v2

HAL Id: hal-01153975

<https://hal.science/hal-01153975v2>

Submitted on 20 Oct 2016

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Preserving monotony of combined edge finite volume–finite element scheme for a bone healing model on general mesh

Marianne Bessemoulin-Chatard* and Mazen Saad†

October 20, 2016

Abstract

In this article, we propose and analyse a combined finite volume–finite element scheme for a bone healing model. This choice of discretization allows to take into account anisotropic diffusions without imposing any restrictions on the mesh. Moreover, following the work of C. Cancès et al. 2013, we define a nonlinear correction of the diffusive terms to obtain a monotone scheme. We provide, under a numerical assumption, a complete convergence analysis of this corrected scheme, and present some numerical experiments which show its good behavior.

Keywords: finite volume scheme; nonconforming finite element scheme; anisotropy; convergence analysis; bone healing model.

1 Introduction

We consider a model taking into account the main biological phenomena acting in bone healing. It describes the evolution of the concentrations of the following four quantities: the mesenchymal stem cells (denoted s), the osteoblasts (denoted b), the bone matrix (denoted m) and the osteogenic growth factor (denoted g). Bone healing begins by the migration of the stem cells to the site of the injury. Then along the bone, these cells differentiate into osteoblasts which start to synthesize the bone matrix. This cell differentiation is only possible in presence of the growth factor.

The proposed model is based on that described in [2]. It takes into account several phenomena: the diffusion of the stem cells and the growth factor, the migration of the stem cells towards the bone matrix, the proliferation and the differentiation of the stem cells. The osteoblasts are considered without movement since they are fixed at the bone matrix. Moreover, the model includes the case of heterogeneous domains, with possibly anisotropic diffusions.

In this paper, we propose and analyse a numerical scheme for this bone growth model. This scheme was already introduced in [4], but without any convergence study. A finite volume scheme was previously proposed in [9] for this model in homogeneous domains where the diffusion tensor is considered to be the identity matrix. Moreover, the convergence analysis is performed only for meshes assumed to be admissible [12, Definition 9.1].

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On the one hand, the classical cell-centered finite volume method with an upwind discretization of the convective terms provides the stability and is extremely robust. In this case, the mesh is assumed to be admissible. In particular, it implies that the orthogonality condition has to be satisfied. As mentioned in [9], a difficulty in the implementation is to construct such admissible meshes. Structured rectangular meshes are admissible, but they cannot be used for complex geometries arising in physical contexts. However, standard finite volume schemes do not permit to handle anisotropic diffusion on general meshes due to the nonconsistency of the numerical flux. A large variety of methods have been proposed to reconstruct a consistent gradient, see for example [13] and references therein.

On the other hand, the finite element method allows for an easy discretization of diffusive terms with full tensors without imposing any restrictions on the meshes. It was used a lot for the discretization of degenerate parabolic equations. For example, conforming piecewise linear finite element method has been studied in [3], as well as mixed finite element method in [1]. However, some numerical instabilities may arise in the convection dominated case.

The idea is hence to combine a finite element discretization of diffusive terms with a finite volume discretization of the other terms. Such schemes were proposed and studied in [15] for fluid mechanics equations where the diffusion tensor is the identity matrix. This method was then extended in [14] to inhomogeneous and anisotropic diffusion–dispersion tensors and to very general meshes only satisfying the shape regularity condition (6). Such discretizations were then applied to different physical models, such as the anisotropic Keller–Segel chemotaxis system [8] or the two compressible phase flow in porous media [17]. However, it is well-known that the discrete maximum principle is no more guaranteed if there exist negative transmissibilities. A nonlinear stabilization term is introduced in [6] to design a Galerkin approximation of the Laplacian, but heterogeneous anisotropic tensors are not considered. More recently, a general approach to construct a nonlinear correction providing a discrete maximum principle was proposed in [7, 16]. This method allows to maintain some crucial properties of the initial scheme, in particular coercivity and convergence toward the weak solution of the continuous problem as the size of the mesh tends to zero. We will apply it to the diffusive terms of our combined scheme to ensure a discrete maximum principle.

The outline of this article is as follows. In Section 2, we introduce the considered bone healing model. In Section 3, we define the combined finite volume–finite element scheme and we apply the method described in [7] to construct a nonlinear correction providing a discrete maximum principle. Then in Section 4 we prove the existence of a physically admissible solution and give some discrete a priori estimates. Thanks to these estimates, we prove in Section 5 the compactness of a family of approximate solutions. It yields the convergence (up to a subsequence) of the solution of the scheme to a solution of the continuous system as the size of the discretization tends to zero. Finally in Section 6 we present some numerical experiments showing the efficiency of the scheme.

2 The bone healing model

We consider the following model for bone healing: for $t \in (0, T)$ and $x \in \Omega$, where $T > 0$ and Ω is an open bounded domain of \mathbb{R}^d ($d = 2, 3$),

$$\partial_t s - \operatorname{div} [\mathbf{D}(x) (\Lambda(m) \nabla s - V(m) \chi(s) \nabla m)] = K_1(m) \chi(s) - H(g) s =: f_1(s, m, g), \quad (1)$$

$$\partial_t b = K_2(m) \chi(b) + \rho H(g) s - \delta_1 b =: f_2(s, b, m, g), \quad (2)$$

$$\partial_t m = \lambda(1 - m) b =: f_3(b, m), \quad (3)$$

$$\partial_t g - \operatorname{div} (\mathbf{D}(x) \Lambda_g \nabla g) = P(g) b - \delta_2 g =: f_4(b, g). \quad (4)$$

The diffusion coefficient $\Lambda(m)$ and haptotaxis velocity $V(m)$ for the stem cells are given by

$$\Lambda(m) = \frac{\chi_h}{\zeta_h^2 + m^2} (m + \lambda_0) (1 - m + \lambda_0), \quad V(m) = \frac{\chi_k}{(\zeta_k + m)^2}.$$

The factors $K_i(m)$, $i = 1, 2$ taking part in the mitosis terms are defined by

$$K_i(m) = \frac{\alpha_i}{\beta_i^2 + m^2} m.$$

The accumulation of stem cells and osteoblasts is limited by the multiplicative term $\chi(s) = s(1 - s)$. Moreover, the differentiation coefficient is given by

$$H(g) = \frac{\gamma_1}{\eta_1 + g} g,$$

and the production term of the growth factor is defined as

$$P(g) = \frac{\gamma_2}{(\eta_2 + g)^2} g.$$

The parameters $\alpha_i, \beta_i, \gamma_i, \eta_i, \delta_i$ ($i = 1, 2$), $\rho, \lambda, \chi_h, \zeta_h, \lambda_0, \chi_k, \zeta_k, \Lambda_g$ are given positive numbers. Finally, we assume that the permeability $\mathbf{D} : \Omega \rightarrow \mathcal{M}_d(\mathbb{R})$, where $\mathcal{M}_d(\mathbb{R})$ is the set of symmetric matrices $d \times d$, verifies:

$$D_{i,j} \in L^\infty(\Omega) \quad \forall i, j = 1, \dots, d,$$

and that there exists $C_D > 0$ such that a.e. $x \in \Omega$, for all $\xi \in \mathbb{R}^d$,

$$\mathbf{D}(x) \xi \cdot \xi \geq C_D |\xi|^2.$$

This diffusion tensor \mathbf{D} allows to take into account the heterogeneity of the biological domain. The system (1)–(4) is supplemented with initial conditions on s, b, m and g :

$$s(0, x) = s_0(x), \quad b(0, x) = b_0(x), \quad m(0, x) = m_0(x), \quad g(0, x) = g_0(x) \quad \forall x \in \Omega,$$

and with homogeneous Neumann boundary conditions on s and g :

$$\mathbf{D}(x) (\Lambda(m) \nabla s - V(m) \chi(s) \nabla m) \cdot \mathbf{n} = 0, \quad \mathbf{D}(x) \Lambda_g \nabla g \cdot \mathbf{n} = 0,$$

for $t \in (0, T)$ and $x \in \partial\Omega$, where \mathbf{n} is the outward unit normal of $\partial\Omega$.

This mathematical model (1)–(4) is studied in [9]. If we denote by $u = (s, b, m, g)$ the unknown and $f : u \in \mathbb{R}^4 \mapsto f(u) = (f_1, f_2, f_3, f_4)(u) \in \mathbb{R}^4$ the reaction term, the following lemma is proved:

Lemma 1. ([9]) *The function f is Lipschitz continuous in the rectangular domain*

$$\mathcal{A} = [0, 1] \times \left[0, \frac{\rho\gamma_1}{\delta_1}\right] \times [0, 1] \times \left[0, \frac{\rho\gamma_1\gamma_2}{4\delta_1\delta_2\eta_2}\right] \quad (5)$$

for $\rho\gamma_1 \geq \delta_1$. Moreover, the domain \mathcal{A} is a contraction set for f , i.e. $f(u) \cdot \mathbf{n} \leq 0$ for all $u \in \partial\mathcal{A}$.

We denote by M_i the upper bound of f_i in \mathcal{A} , $i = 1, \dots, 4$. In the rest of this paper, we will assume that $\rho\gamma_1 \geq \delta_1$, which ensures the invariance of the domain \mathcal{A} of admissible solutions, defined as follows:

Definition 1 (Admissible weak solutions). *Let (s_0, b_0, m_0, g_0) belongs to \mathcal{A} almost everywhere in Ω . A function $u = (s, b, m, g) \in (L^2(0, T; H^1(\Omega)))^4$ is a weak admissible solution of (1)–(4) if $u(t, x) \in \mathcal{A}$ a.e. in $Q_T := (0, T) \times \Omega$ and if for any test functions $\varphi_1, \varphi_2, \varphi_3$ and $\varphi_4 \in C_c^\infty([0, T) \times \overline{\Omega})$, the function u satisfies the following equalities:*

$$\begin{aligned} & - \int_{Q_T} s \partial_t \varphi_1 dx dt - \int_{\Omega} s_0(x) \varphi_1(0, x) dx + \int_{Q_T} \mathbf{D}(x) (\Lambda(m) \nabla s - V(m) \chi(s) \nabla m) \cdot \nabla \varphi_1 dx dt = \\ & \quad \int_{Q_T} f_1(s, m, g) \varphi_1 dx dt, \\ & - \int_{Q_T} b \partial_t \varphi_2 dx dt - \int_{\Omega} b_0(x) \varphi_2(0, x) dx = \int_{Q_T} f_2(s, b, m, g) \varphi_2 dx dt, \\ & - \int_{Q_T} m \partial_t \varphi_3 dx dt - \int_{\Omega} m_0(x) \varphi_3(0, x) dx = \int_{Q_T} f_3(b, m) \varphi_3 dx dt, \\ & - \int_{Q_T} g \partial_t \varphi_4 dx dt - \int_{\Omega} g_0(x) \varphi_4(0, x) dx + \int_{Q_T} \mathbf{D}(x) \Lambda_g \nabla g \cdot \nabla \varphi_4 dx dt = \int_{Q_T} f_4(b, g) \varphi_4 dx dt. \end{aligned}$$

3 Combined finite volume-nonconforming finite element scheme

In this section, we first introduce the primal triangulation and the corresponding dual partition of the domain Ω , and then define our numerical scheme.

3.1 Space and time discretization

We first define the space discretization of Ω . We consider a family \mathcal{T}_h of meshes of Ω , consisting of closed simplices K with disjoint interiors such that $\overline{\Omega} = \cup_{K \in \mathcal{T}_h} K$ and such that if $K, L \in \mathcal{T}_h$, $K \neq L$, then $K \cap L$ is either an empty set or a common edge of K and L . The size of the mesh \mathcal{T}_h is defined by

$$h := \text{size}(\mathcal{T}_h) = \max_{K \in \mathcal{T}_h} \text{diam}(K).$$

We also need the following regularity assumption on the family of triangulations $\{\mathcal{T}_h\}_h$: there exists a positive constant $k_{\mathcal{T}}$ such that:

$$\min_{K \in \mathcal{T}_h} \frac{|K|}{(\text{diam}(K))^d} \geq k_{\mathcal{T}}, \quad \forall h > 0. \quad (6)$$

We denote by:

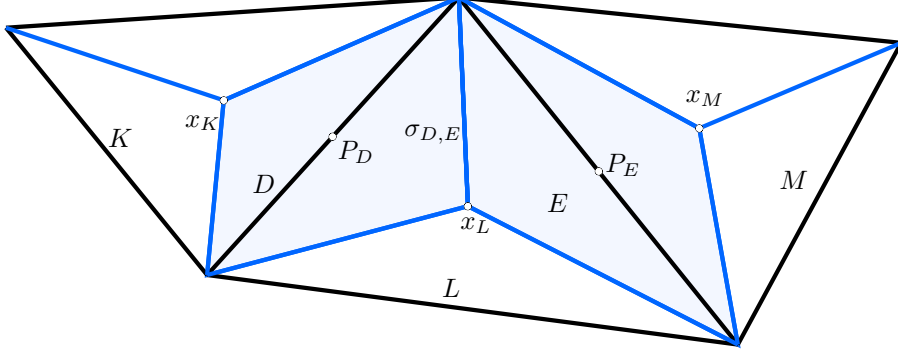


Figure 1: Triangles K, L and $M \in \mathcal{T}_h$ and diamonds $D, E \in \mathcal{D}_h$ associated with edges $\sigma_D, \sigma_E \in \mathcal{E}_h$.

- \mathcal{E}_h the set of all edges, $\mathcal{E}_h = \mathcal{E}_h^{int} \cup \mathcal{E}_h^{ext}$ where \mathcal{E}_h^{int} is the set of interior edges and \mathcal{E}_h^{ext} the set of boundary edges,
- \mathcal{E}_K the set of all edges of an element $K \in \mathcal{T}_h$.

We also use a dual partition \mathcal{D}_h , called diamond mesh, of control volumes D of Ω such that $\overline{\Omega} = \cup_{D \in \mathcal{D}_h} D$. Each diamond D is associated with one edge $\sigma_D \in \mathcal{E}_h$. We construct it by connecting the barycenters of every $K \in \mathcal{T}_h$ that contains σ_D through the vertices of σ_D (see Figure 3.1). For $\sigma_D \in \mathcal{E}_h^{ext}$, the contour of D is completed by the edge σ_D itself. In this case, the diamond D is in fact a half diamond. As for the primal mesh, we define:

- $\mathcal{F}_h, \mathcal{F}_h^{int}$ and \mathcal{F}_h^{ext} respectively as the set of all dual, interior dual and exterior dual mesh edges,
- \mathcal{D}_h^{int} and \mathcal{D}_h^{ext} respectively as the set of all interior and boundary diamonds.

In the sequel, we also use the following notations:

- $|D|$ is the d -dimensional Lebesgue measure of D , $|\sigma|$ the $(d-1)$ -dimensional measure of σ ,
- P_D is the barycenter of the edge σ_D ,
- $\mathcal{N}(D)$ is the set of neighbours of the volume D ,
- $\mathcal{D}_K := \{D \in \mathcal{D}_h, \sigma_D \in \mathcal{E}_K\}$ for $K \in \mathcal{T}_h$.

For two neighbouring diamonds $D \in \mathcal{D}_h$ and $E \in \mathcal{N}(D)$, we define:

- $d_{D,E} := |P_E - P_D|$,
- $\sigma_{D,E} = \partial D \cap \partial E$ the interface between the two diamonds D and E ,

- $\mathbf{n}_{D,E}$ the unit normal vector to $\sigma_{D,E}$ outward to D ,
- $K_{D,E}$ the unique element of \mathcal{T}_h such that $\sigma_{D,E} \subset K_{D,E}$, namely the unique triangle $K_{D,E}$ such that $K_{D,E} \cap D \neq \emptyset$ and $K_{D,E} \cap E \neq \emptyset$.

We denote by $X(\mathcal{D}_h)$ the set of finite volume approximations on the diamond mesh \mathcal{D}_h , that is the set of piecewise constant functions on the control volumes $D \in \mathcal{D}_h$.

Next we define the following piecewise linear nonconforming finite element space (see [10]):

$$X_h := \{\varphi_h \in L^2(\Omega); \varphi_h|_K \text{ is linear } \forall K \in \mathcal{T}_h, \varphi_h \text{ is continuous at points } P_D, D \in \mathcal{D}_h^{int}\}.$$

The basis of the nonconforming space X_h is spanned by the shape functions φ_D , $D \in \mathcal{D}_h$, such that $\varphi_D(P_E) = \delta_{DE}$, $E \in \mathcal{D}_h$, where $\delta_{D,E}$ is Kronecker's symbol. We equip X_h with the seminorm

$$\|u_h\|_{X_h}^2 := \sum_{K \in \mathcal{T}_h} \int_K |\nabla u_h|^2 dx.$$

We refer to [14] for the following properties : for all $u_h = \sum_{D \in \mathcal{D}_h} u_D \varphi_D \in X_h$, it holds

$$\sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \text{diam}(K_{D,E})^{d-2} (u_E - u_D)^2 \leq \frac{d+1}{2dk_{\mathcal{T}}} \|u_h\|_{X_h}^2, \quad (7)$$

$$\sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \frac{|\sigma_{D,E}|}{d_{D,E}} (u_E - u_D)^2 \leq \frac{d+1}{2(d-1)k_{\mathcal{T}}} \|u_h\|_{X_h}^2. \quad (8)$$

Let us now define the time discretization. We consider a constant time step Δt and the increasing sequence $(t^n)_{0 \leq n \leq N+1}$, where $t^n = n \Delta t$ and N is the smallest integer such that $(N+1)\Delta t \geq T$. At last, the size of the space-time discretization is defined by $\Delta := \max(h, \Delta t)$.

The discrete unknowns are denoted by $\{v_D^n, D \in \mathcal{D}_h, n \in \{0, \dots, N+1\}\}$, where the value v_D^n is an approximation of $v(P_D, t^n)$, $v = s, b, m, g$.

3.2 Combined scheme

In this subsection, we define the semi-implicit in time and combined finite volume–finite element in space discretization for (1)–(4). On the one hand, the haptotaxis term in the stem cell equation (1) can be seen as a convection term with velocity $V(m)\nabla m$, and is discretized by the mean of a classical upwind finite volume approach. On the other hand, the diffusive terms in equations (1) and (4) are discretized by using a finite element scheme, which enables to get a consistent approximation, even in the homogeneous case $\mathbf{D} = Id$. Hence this numerical scheme allows to consider both general meshes and anisotropic diffusion tensors.

First of all, the discrete initial condition is defined by:

$$\forall D \in \mathcal{D}_h, \quad v_D^0 = \frac{1}{|D|} \int_D v_0(x) dx, \quad \text{for } v = s, b, m, g.$$

Then the scheme is given by the following set of equations: for all $n \in \{0, \dots, N\}$ and all $D \in \mathcal{D}_h$,

$$\begin{aligned} |D| (s_D^{n+1} - s_D^n) - \Delta t \sum_{E \in \mathcal{D}_h} \Lambda_{D,E}^{n+1} s_E^{n+1} + \Delta t \sum_{E \in \mathcal{N}(D)} F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1})) \\ = \Delta t |D| (K_1(m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1}), \end{aligned} \quad (9)$$

$$|D| (b_D^{n+1} - b_D^n) = \Delta t |D| f_2(s_D^{n+1}, b_D^{n+1}, m_D^n, g_D^n), \quad (10)$$

$$|D| (m_D^{n+1} - m_D^n) = \Delta t |D| f_3(b_D^{n+1}, m_D^{n+1}), \quad (11)$$

$$|D| (g_D^{n+1} - g_D^n) - \Delta t \sum_{E \in \mathcal{D}_h} \mathcal{D}_{D,E} \Lambda_g g_E^{n+1} = \Delta t |D| (P(g_D^n) b_D^n - \delta_2 g_D^{n+1}), \quad (12)$$

where the stiffness coefficient is defined as

$$\mathcal{D}_{D,E} = - \sum_{K \in \mathcal{T}_h} \int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D dx,$$

and for $U = \Lambda, V$,

$$D, E = - \sum_{K \in \mathcal{T}_h} U_K \int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D dx, \quad (13)$$

with

$$U_K = \frac{\sum_{D \in \mathcal{D}_K} U(m_D)}{\text{card}(\mathcal{D}_K)}.$$

As proved in [8, Lemma 4.2], the transmissibilities $\mathcal{D}_{D,E}$ are bounded:

$$|\mathcal{D}_{D,E}| \leq \frac{c_D}{k_{\mathcal{T}}} \frac{(\text{diam}(K_{D,E}))^{d-2}}{(d-1)^2}, \quad \forall D \in \mathcal{D}_h, \quad E \in \mathcal{N}(D). \quad (14)$$

An approximation of $\mathbf{D}(x) V(m) \chi(s) \nabla m \cdot \mathbf{n}_{D,E}$ at the interface $\sigma_{D,E}$ is given by

$$F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1})), \quad (15)$$

where the flux function F is supposed to satisfy the following properties:

- **monotony**: for all $(a, c) \in \mathbb{R}^2$, $b \mapsto F(a, b, c)$ is nonincreasing,
- **consistency**: for all $(a, c) \in \mathbb{R}^2$, we have $F(a, a, c) = c \chi(a)$,
- **conservativity**: for all $(a, b, c) \in \mathbb{R}^3$ we have $F(a, b, c) = -F(b, a, -c)$,
- **local Lipschitz continuity**: given $M \in \mathbb{R}$, there exists $L_M > 0$ such that for all $c \in \mathbb{R}$ and $(a, b), (a', b') \in \mathbb{R}^2$ such that $\max(|a|, |b|, |a'|, |b'|) \leq M$, we have

$$|F(a, b, c) - F(a', b', c)| \leq L_M |c| (|a - a'| + |b - b'|).$$

For example, we consider in the following the Osher numerical flux function defined by

$$F(a, b, c) = c^+ (\chi_{\uparrow}(a) + \chi_{\downarrow}(b)) - c^- (\chi_{\uparrow}(b) + \chi_{\downarrow}(a)),$$

where $c^+ = \max(c, 0)$, $c^- = \max(-c, 0)$, χ_\uparrow and χ_\downarrow are respectively the nondecreasing and nonincreasing parts of χ :

$$\chi_\uparrow(a) := \int_0^a (\chi'(z))^+ dz, \quad \chi_\downarrow(a) := - \int_0^a (\chi'(z))^- dz.$$

Definition 2 (Approximate solutions). *Using the values $(v_D^{n+1})_{D \in \mathcal{D}_h, n \in \{0, \dots, N\}}$, $v = s, b, m, g$, we define two approximate solutions by mean of the combined finite volume-nonconforming finite element scheme:*

- *a nonconforming finite element solution v_Δ as a function piecewise linear and continuous in the barycenters of interior edges in space and piecewise constant in time, such that*

$$v_\Delta(t, x) = v_h^{n+1}(x) = \sum_{D \in \mathcal{D}_h} v_D^{n+1} \varphi_D(x), \quad x \in \Omega, t \in (t^n, t^{n+1}],$$

- *a finite volume solution \bar{v}_Δ defined as piecewise constant on the diamonds in space and piecewise constant in time, such that*

$$\bar{v}_\Delta(t, x) = \bar{v}_h^{n+1}(x) = v_D^{n+1}, \quad x \in D, t \in (t^n, t^{n+1}].$$

We also define \tilde{v}_Δ as the function piecewise constant on the simplices $K \in \mathcal{T}_h$ and piecewise constant in time such that

$$\tilde{v}_\Delta(t, x) = \tilde{v}_h^{n+1}(x) = v_K^{n+1} := \frac{1}{\text{Card}(\mathcal{D}_K)} \sum_{E \in \mathcal{D}_K} v_E^{n+1}, \quad x \in K, t \in (t^n, t^{n+1}]. \quad (16)$$

3.3 Monotone correction

At this stage, the constructed scheme is valid both for full anisotropic diffusion tensors and for general meshes satisfying only assumption (6). However, it possesses a discrete maximum principle only if all transmissibilities coefficients $\Lambda_{D,E}$, $\mathcal{D}_{D,E}$, $E \in \mathcal{N}(D)$, $E \neq D$, are nonnegative, which is not guaranteed in the general case. In the isotropic case and for a pure finite volume scheme on orthogonal mesh, the authors show in [9] the maximum principle and the convergence of the finite volume scheme.

Following [7], we now define a nonlinear correction which ensures monotony while preserving the main properties of the original discrete diffusive operators (conservativity, coercivity, continuity) as detailed in Section 4.1. We first explain briefly the construction of the monotone correction for the following elliptic equation:

$$-\text{div}(\mathbf{D}(x)\nabla u) = f,$$

with homogeneous Dirichlet boundary conditions. We consider a discretization of this equation written in a conservative form as:

$$S_D(u_h) = \sum_{D \in \mathcal{D}_h} \sum_{\sigma \in \mathcal{F}_D} \tau_{D,\sigma} (u_D - u_{D,\sigma}) = f_D, \quad \forall D \in \mathcal{D}_h,$$

where

$$u_{D,\sigma} = \begin{cases} u_E & \text{if } \sigma = \sigma_{D,E} \in \mathcal{F}_h^{int}, \\ 0 & \text{if } \sigma \in \mathcal{F}_h^{ext}. \end{cases}$$

The scheme is monotone if all the transmissibility coefficients $\tau_{D,\sigma}$ are positive. In the case where the positiveness of these coefficients is not satisfied, the correction consists in adding an artificial discrete diffusion to require the monotony of the corrected scheme. More precisely, the idea is to choose a family $(\beta_{D,\sigma})$ such that the corrected operator defined by:

$$\Sigma_D(u_h) = S_D(u_h) + \sum_{D \in \mathcal{D}_h} \sum_{\sigma \in \mathcal{F}_D} \beta_{D,\sigma} (u_D - u_{D,\sigma})$$

is monotone [7]. We now detail this construction in our case.

Let us define

$$\mathcal{S}^{\mathcal{D}_h} : \begin{array}{ccc} \mathbb{R}^{Card(\mathcal{D}_h)} & \rightarrow & \mathbb{R}^{Card(\mathcal{D}_h)} \\ s_h = (s_D)_{D \in \mathcal{D}_h} & \mapsto & (S_D(s_h))_{D \in \mathcal{D}_h} \end{array}, \quad \mathcal{G}^{\mathcal{D}_h} : \begin{array}{ccc} \mathbb{R}^{Card(\mathcal{D}_h)} & \rightarrow & \mathbb{R}^{Card(\mathcal{D}_h)} \\ g_h = (g_D)_{D \in \mathcal{D}_h} & \mapsto & (G_D(g_h))_{D \in \mathcal{D}_h} \end{array},$$

the original discrete diffusive operators appearing in (9) and (12), with for all $D \in \mathcal{D}_h$,

$$S_D(s_h) = - \sum_{E \in \mathcal{D}_h} \Lambda_{D,E} s_E, \quad G_D(g_h) = - \sum_{E \in \mathcal{D}_h} \Lambda_g \mathcal{D}_{D,E} g_E.$$

We replace the diffusive operator $\mathcal{S}^{\mathcal{D}_h}$ in (9) by the corrected operator $\mathbb{S}^{\mathcal{D}_h}$, for which the coordinate D is defined by:

$$\Sigma_D(s_h) = S_D(s_h) + \sum_{E \in \mathcal{N}(D)} \mathfrak{s}_{D,E}(s_h)(s_D - s_E) \quad \forall D \in \mathcal{D}_h,$$

where the correction $(\mathfrak{s}_{D,E}(s_h))_{D \in \mathcal{D}_h, E \in \mathcal{N}(D)}$ satisfies the following properties (see [7]):

(P1) Let $(\gamma_{D,E})_{D \in \mathcal{D}_h, E \in \mathcal{N}(D)}$ be a family of functions $\gamma_{D,E} : \mathbb{R}^{Card(\mathcal{D}_h)} \rightarrow \mathbb{R}_+$ such that for all $s_h = (s_D)_{D \in \mathcal{D}_h} \in \mathbb{R}^{Card(\mathcal{D}_h)}$, for all $D \in \mathcal{D}_h$,

$$\text{if } \sum_{E \in \mathcal{N}(D)} |s_D - s_E| \neq 0, \text{ then } \sum_{E \in \mathcal{N}(D)} \gamma_{D,E}(s_h) |s_D - s_E| = 1. \quad (17)$$

We assume that

$$\forall D \in \mathcal{D}_h, \quad \forall E \in \mathcal{N}(D), \quad \mathfrak{s}_{D,E} > \gamma_{D,E}(s_h) |S_D(s_h)|. \quad (18)$$

More precisely, we consider corrections which can be written under the form

$$\mathfrak{s}_{D,E} = \alpha \gamma_{D,E}(s_h) |S_D(s_h)| + \frac{|\sigma_{D,E}|}{d_{D,E}}, \quad \alpha \geq 1. \quad (19)$$

(P2) The family $(\mathfrak{s}_{D,E}(s_h))_{D \in \mathcal{D}_h, E \in \mathcal{N}(D)}$ is symmetric:

$$\forall D \in \mathcal{D}_h, \quad \forall E \in \mathcal{N}(D), \quad \mathfrak{s}_{D,E} = \mathfrak{s}_{E,D}.$$

(P3) Let $(\mathcal{D}_h)_h$ be a sequence of diamond meshes discretizing Ω . Let $(\mathbb{S}^{\mathcal{D}_h})_h$ be a sequence of associated corrections. We assume that

$$\sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \text{diam}(D) \sum_{E \in \mathcal{N}(D)} \mathfrak{s}_{D,E}(s_h^{n+1}) |s_D^{n+1} - s_E^{n+1}| \rightarrow 0 \text{ as } \Delta t, h \rightarrow 0. \quad (20)$$

The property (P1) ensures the monotony, whereas the property (P2) guarantees the conservativity of the numerical fluxes. Finally, the property (P3) ensures that the additional diffusion does not jeopardize the convergence of the corrected scheme. According to [7, Remark 3.5], for a convenient choice of the correction, we can deduce this property from the energy estimate on the discrete gradient of the solution (see Proposition 2).

The diffusive operator $\mathcal{G}^{\mathcal{D}_h}$ in (12) can also be corrected in the same way by $\mathbb{G}^{\mathcal{D}_h}$ given by

$$\Gamma_D(g_h) = G_D(g_h) + \sum_{E \in \mathcal{N}(D)} \mathfrak{g}_{D,E}(g_h)(g_D - g_E) \quad \forall D \in \mathcal{D}_h,$$

where $\mathfrak{g}_{D,E}$ satisfies the same properties as $\mathfrak{s}_{D,E}$.

Examples of such corrections can be found in [7]. In our numerical experiments, we use the regularized correction defined by:

$$\mathfrak{s}_{D,E}(s) = \max \left(\frac{|S_D(s)|}{\text{Card}_\varepsilon V(D, s)^\star}, \frac{|S_E(s)|}{\text{Card}_\varepsilon V(E, s)^\star} \right) \frac{1}{|s_D - s_E| + \varepsilon} + \frac{|\sigma_{D,E}|}{d_{D,E}},$$

where

$$\text{Card}_\varepsilon V(D, s)^\star = \sum_{E \in \mathcal{N}(D)} \frac{|s_D - s_E|}{|s_D - s_E| + \varepsilon}.$$

It is clear that the assumption (19) is verified by this particular example. Concerning condition (20), it can be verified numerically as detailed in [7] and [8].

In the sequel, we always assume that stated properties on the numerical flux F defined by (15) and on the corrections $\mathfrak{s}_{D,E}$ and $\mathfrak{g}_{D,E}$ are fulfilled.

4 Properties of the scheme

4.1 Some preliminary results

We first present some properties of the original discrete diffusive operators $\mathcal{S}^{\mathcal{D}_h}$ and $\mathcal{G}^{\mathcal{D}_h}$.

- **Conservativity.** It can be easily proved (see [14, Lemma 4.1]) that for all $D \in \mathcal{D}_h$, one has

$$\Lambda_{D,D} = - \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E},$$

Then using the fact that $\Lambda_{D,E} \neq 0$ only if $E \in \mathcal{N}(D)$ or if $E = D$, we have:

$$S_D(v_h) = \sum_{E \in \mathcal{D}_h} \Lambda_{D,E} v_E = \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E} v_E + \Lambda_{D,D} v_D = \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E} (v_E - v_D). \quad (21)$$

Writing

$$S_D(v_h) = \sum_{E \in \mathcal{N}(D)} \mathcal{F}_{D,E}^S$$

since \mathbf{D} is symmetric, the numerical flux is conservative:

$$\mathcal{F}_{D,E}^S + \mathcal{F}_{E,D}^S = 0.$$

In the same way,

$$G_D(v_h) = \sum_{E \in \mathcal{N}(D)} \Lambda_g \mathcal{D}_{D,E}(v_D - v_E) = \sum_{E \in \mathcal{N}(D)} \mathcal{F}_{D,E}^G,$$

and the numerical flux satisfies:

$$\mathcal{F}_{D,E}^G + \mathcal{F}_{E,D}^G = 0.$$

- **Coercivity.** Assuming that $\Lambda_K \geq \Lambda_0 > 0$, using the definition of $\Lambda_{D,E}$ and the coercivity of the tensor \mathbf{D} , we have:

$$\begin{aligned} \sum_{D \in \mathcal{D}_h} S_D(v_h) v_D &= \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \sum_{K \in \mathcal{T}_h} \Lambda_K \left(\int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D \right) v_E v_D \\ &= \sum_{K \in \mathcal{T}_h} \Lambda_K \left(\int_K \mathbf{D}(x) \nabla v_h \cdot \nabla v_h \right) \geq \Lambda_0 C_D \|v_h\|_{X_h}^2 = C_S \|v_h\|_{X_h}^2. \end{aligned} \quad (22)$$

There also exists $C_G > 0$ such that

$$\sum_{D \in \mathcal{D}_h} G_D(v_h) v_D \geq C_G \|v_h\|_{X_h}^2.$$

We now present the properties of the corrected operators $\mathbb{S}^{\mathcal{D}_h}$ and $\mathbb{G}^{\mathcal{D}_h}$. Using property (P2), their conservativity is an easy consequence of the conservativity of $\mathcal{S}^{\mathcal{D}_h}$, $\mathcal{G}^{\mathcal{D}_h}$. The coercivity stems from the coercivity of $\mathcal{S}^{\mathcal{D}_h}$ and $\mathcal{G}^{\mathcal{D}_h}$ and the nonnegativity of $\mathfrak{s}_{D,E}$, $\mathfrak{g}_{D,E}$ for all $D \in \mathcal{D}_h$, $E \in \mathcal{N}(D)$. Moreover, $\mathbb{S}^{\mathcal{D}_h}$ and $\mathbb{G}^{\mathcal{D}_h}$ are **monotone**, in the sense that for all $v_h \in X_h$, for all $D \in \mathcal{D}_h$, $\Sigma_D(v_h)$ and $\Gamma_D(v_h)$ can be written under the form

$$\Sigma_D(v_h) = \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}(v_h)(v_D - v_E), \quad (23)$$

$$\Gamma_D(v_h) = \sum_{E \in \mathcal{N}(D)} \mathbb{G}_{D,E}(v_h)(v_D - v_E), \quad (24)$$

where the functions $\mathbb{S}_{D,E}, \mathbb{G}_{D,E} : \mathbb{R}^{Card(\mathcal{D}_h)} \rightarrow \mathbb{R}_+$ satisfy the following property:

$$\mathbb{S}_{D,E}(v_h) > 0, \quad \mathbb{G}_{D,E}(v_h) > 0, \quad \forall v_h \in \mathbb{R}^{Card(\mathcal{D}_h)}.$$

In fact, using (21),

$$\mathbb{S}_{D,E}(v_h) = \Lambda_{D,E} + \mathfrak{s}_{D,E}(v_h). \quad (25)$$

It remains to see that $\mathbb{S}_{D,E}(v_h) > 0$. To this end, we follow the same proof as in [7, Proposition 3.1]. Using (17), we can write

$$\begin{aligned} S_D(v_h) &= \sum_{E \in \mathcal{N}(D)} \gamma_{D,E}(v_h) |v_D - v_E| S_D(v_h) \\ &= \sum_{E \in \mathcal{N}(D)} [\gamma_{D,E}(v_h) \text{sgn}(v_D - v_E) S_D(v_h)] (v_D - v_E). \end{aligned}$$

Then the coordinate D of the corrected operator $\mathbb{S}^{\mathcal{D}_h}$ can be written under the form (23), with

$$\mathbb{S}_{D,E}(v_h) = \gamma_{D,E}(v_h) \text{sgn}(v_D - v_E) S_D(v_h) + \mathfrak{s}_{D,E}(v_h). \quad (26)$$

Using (18), it is clear that $\mathbb{S}_{D,E}(v_h) > 0$. Similarly, one gets $\mathbb{G}_{D,E}(v_h) > 0$.

Remark 1. Combining (25) and (26), we obtain that

$$\Lambda_{D,E} = \gamma_{D,E}(s_h) \operatorname{sgn}(s_D - s_E) S_D(s_h),$$

and finally

$$|\Lambda_{D,E}| = \gamma_{D,E}(s_h) |S_D(s_h)|, \quad (27)$$

which will be useful later.

Summarizing, the corrected scheme that will be studied in the following is:

$$\begin{aligned} |D| (s_D^{n+1} - s_D^n) - \Delta t \sum_{E \in \mathcal{D}_h} \mathbb{S}_{D,E}^{n+1} s_E^{n+1} + \Delta t \sum_{E \in \mathcal{N}(D)} F \left(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1}) \right) \\ = \Delta t |D| (K_1(m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1}), \end{aligned} \quad (28)$$

$$|D| (b_D^{n+1} - b_D^n) = \Delta t |D| f_2(s_D^{n+1}, b_D^{n+1}, m_D^n, g_D^n), \quad (29)$$

$$|D| (m_D^{n+1} - m_D^n) = \Delta t |D| f_3(b_D^{n+1}, m_D^{n+1}), \quad (30)$$

$$|D| (g_D^{n+1} - g_D^n) - \Delta t \sum_{E \in \mathcal{D}_h} \mathbb{G}_{D,E}^{n+1} g_E^{n+1} = \Delta t |D| (P(g_D^n) b_D^n - \delta_2 g_D^{n+1}). \quad (31)$$

4.2 Existence of a physically admissible discrete solution

As in [9], we introduce the following truncated version of the discrete system (28)–(31) to prove the existence of a discrete admissible solution:

$$\begin{aligned} |D| (s_D^{n+1} - s_D^n) - \Delta t \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) + \\ \Delta t \sum_{E \in \mathcal{N}(D)} \tilde{F} \left(s_D^{n+1}, s_E^{n+1}, \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right) = \\ \Delta t |D| (K_1(m_D^n) \tilde{s}_D^{n+1} (1 - s_D^n) - H(g_D^n) \tilde{s}_D^{n+1}), \end{aligned} \quad (32)$$

$$|D| (b_D^{n+1} - b_D^n) = \Delta t |D| f_2 \left(\tilde{s}_D^{n+1}, \tilde{b}_D^{n+1}, m_D^n, g_D^n \right), \quad (33)$$

$$|D| (m_D^{n+1} - m_D^n) = \Delta t |D| f_3 \left(\tilde{b}_D^{n+1}, \tilde{m}_D^{n+1} \right), \quad (34)$$

$$|D| (g_D^{n+1} - g_D^n) - \Delta t \sum_{E \in \mathcal{N}(D)} \mathbb{G}_{D,E}^{n+1} (g_E^{n+1} - g_D^{n+1}) = \Delta t |D| (P(g_D^n) b_D^n - \delta_2 \tilde{g}_D^{n+1}), \quad (35)$$

where we use the general truncation function $Z_{[a,b]}(r) = \min(b, \max(a, r))$ and some truncation associated to the definition of the admissibility region \mathcal{A} as follows

$$\tilde{s} = Z_{[0,1]}(s), \quad \tilde{b} = Z_{[0, \rho \frac{\gamma_1}{\delta_1}]}(b), \quad \tilde{m} = Z_{[0,1]}(m), \quad \tilde{g} = Z_{[0, \frac{\rho \gamma_1 \gamma_2}{4 \delta_1 \delta_2}]}(g),$$

$$\tilde{V}_{DE} = - \sum_{K \in \mathcal{T}_h} \tilde{V}_K \int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D,$$

with

$$\tilde{V}_K = \frac{\sum_{D \in \mathcal{D}_K} V(\tilde{m}_D)}{\text{card}(\mathcal{D}_K)}.$$

Furthermore, the flux function \tilde{F} is defined like F after replacing χ by $\chi \circ Z_{[0,1]}$. It is easy to see that \tilde{F} satisfies the same properties as F (monotony, consistency, conservativity, local Lipschitz continuity). Moreover, for all $(a, b, c) \in \mathbb{R}^3$,

$$|\tilde{F}(a, b, c)| \leq |c| \int_0^1 |\chi'(s)| ds =: |c| c_0, \quad (36)$$

and for all $a, b \in [0, 1]$, $c \in \mathbb{R}$,

$$\tilde{F}(a, b, c) = F(a, b, c).$$

To prove the existence of an admissible discrete solution, we follow the same reasoning as in [9]. Indeed, we first establish the result for the truncated system (32)–(35). More precisely, we will now prove the following lemmas and existence theorem.

Lemma 2. *Given any $(s_D^n, b_D^n, m_D^n, g_D^n)_{D \in \mathcal{D}_h}$, the truncated system (32)–(35) admits at least one solution $(s_D^{n+1}, b_D^{n+1}, m_D^{n+1}, g_D^{n+1})_{D \in \mathcal{D}_h}$.*

Proof. We apply the following result, which is proved for example in [18, Lemma 1.4, Chapter II]

Lemma 3. *(see [18]) Let X be a finite dimensional Hilbert space with scalar product $(\cdot, \cdot)_X$ and associated norm $\|\cdot\|_X$. Let $P : X \rightarrow X$ be a continuous mapping such that $(P(\xi), \xi)_X > 0$ for all $\xi \in X$ such that $\|\xi\|_X = k$, for some fixed $k > 0$. Then there exists $\xi_0 \in X$ such that $\|\xi_0\|_X \leq k$ and $P(\xi_0) = 0$.*

We apply this result with $X = (X(\mathcal{D}_h))^4$ for P that maps $\bar{u}_h^{n+1} = (\bar{s}_h^{n+1}, \bar{b}_h^{n+1}, \bar{m}_h^{n+1}, \bar{g}_h^{n+1})$ to the left-hand sides minus the right-hand sides of (32)–(35) for all $D \in \mathcal{D}_h$. The inner product is

$$(\bar{u}_h^1, \bar{u}_h^2)_X = (\bar{s}_h^1, \bar{s}_h^2)_{L^2} + (\bar{b}_h^1, \bar{b}_h^2)_{L^2} + (\bar{m}_h^1, \bar{m}_h^2)_{L^2} + (\bar{g}_h^1, \bar{g}_h^2)_{L^2}$$

for any $\bar{u}_h^i = (\bar{s}_h^i, \bar{b}_h^i, \bar{m}_h^i, \bar{g}_h^i) \in X$, $i = 1, 2$.

We have to prove that $(P(\bar{u}_h^{n+1}), \bar{u}_h^{n+1})_X > 0$ for all \bar{u}_h^{n+1} large enough. We have

$$(P(\bar{u}_h^{n+1}), \bar{u}_h^{n+1})_X = A_1 + A_2 + A_3 + A_4,$$

where

$$\begin{aligned} A_1 &= \sum_{D \in \mathcal{D}_h} |D| ((s_D^{n+1} - s_D^n) s_D^{n+1} + (b_D^{n+1} - b_D^n) b_D^{n+1} + (m_D^{n+1} - m_D^n) m_D^{n+1} + (g_D^{n+1} - g_D^n) g_D^{n+1}), \\ A_2 &= -\Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \left(\mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) s_D^{n+1} + \mathbb{G}_{D,E}^{n+1} (g_E^{n+1} - g_D^{n+1}) g_D^{n+1} \right), \\ A_3 &= \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \tilde{F} \left(s_D^{n+1}, s_E^{n+1}, \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right) s_D^{n+1}, \\ A_4 &= -\Delta t \sum_{D \in \mathcal{D}_h} |D| \left[s_D^{n+1} (K_1(m_D^n) \tilde{s}_D^{n+1} (1 - s_D^n) - H(g_D^n) \tilde{s}_D^{n+1}) \right. \\ &\quad \left. + b_D^{n+1} f_2(\tilde{s}_D^{n+1}, \tilde{b}_D^{n+1}, \tilde{m}_D^{n+1}, \tilde{g}_D^{n+1}) + m_D^{n+1} f_3(\tilde{b}_D^{n+1}, \tilde{m}_D^{n+1}) + g_D^{n+1} (P(g_D^n) b_D^n - \delta_2 \tilde{g}_D^{n+1}) \right]. \end{aligned}$$

- Using the inequality $(a - b)a \geq \frac{1}{2}(a^2 - b^2)$, we obtain that

$$A_1 \geq \frac{1}{2} (\|\bar{u}_h^{n+1}\|_X^2 - \|\bar{u}_h^n\|_X^2).$$

- Using the conservativity of the discrete corrected diffusive operators, we have:

$$A_2 = -\Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \left(\mathbb{S}_{D,E}^{n+1} s_E^{n+1} s_D^{n+1} + \mathbb{G}_{D,E}^{n+1} g_E^{n+1} g_D^{n+1} \right),$$

and then using their coercivity, we finally obtain:

$$A_2 \geq \Delta t (C_S \|s_h^{n+1}\|_{X_h}^2 + C_G \|g_h^{n+1}\|_{X_h}^2) \geq 0.$$

- To bound A_3 , firstly remark, since $0 \leq \tilde{m}_D^{n+1} \leq 1$, that

$$\left| \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right| \leq \left| \tilde{V}_{D,E}^{n+1} \right|.$$

Then we have

$$\left| \tilde{V}_{D,E}^{n+1} \right| = \left| \sum_{K \in \mathcal{T}_h} \tilde{V}_K^{n+1} \left(\int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D \right) \right| = \left| \tilde{V}_{K_{D,E}}^{n+1} (\mathbf{D}(x) \nabla \varphi_E, \nabla \varphi_D)_{0,K_{D,E}} \right|$$

Since $m \mapsto V(m)$ is a nonnegative decreasing function for $m \in [0, 1]$, using assumption (6) and following the same computations as in [8, Lemma 4.2], we get

$$\left| \tilde{V}_{D,E}^{n+1} \right| \leq V(0) \frac{c_D}{k_{\mathcal{T}}} \frac{\text{diam}(K_{D,E})^{d-2}}{(d-1)^2}.$$

Finally, using the estimate (36) and the above estimate, it yields

$$\begin{aligned} A_3 &\geq -\Delta t |c_0| V(0) \frac{c_D}{k_{\mathcal{T}}} \max_{D \in \mathcal{D}_h} \left(\frac{1}{|D|} \sum_{E \in \mathcal{N}(D)} \frac{\text{diam}(K_{D,E})^{d-2}}{(d-1)^2} \right) \sum_{D \in \mathcal{D}_h} |D| |s_D^{n+1}| \\ &\geq -C_1 \|\bar{s}_h^{n+1}\|_{L^2} \geq -C_1 \|\bar{u}_h^{n+1}\|_X. \end{aligned}$$

- Concerning A_4 , we use the continuity of the functions K_1 , H , f_2 , f_3 , P , and the boundedness of $(\bar{u}_D^{n+1})_{D \in \mathcal{D}_h}$, $(u_D^n)_{D \in \mathcal{D}_h} \in \mathcal{A}$ to obtain that

$$A_4 \geq -C_2 \|\bar{u}_h^{n+1}\|_X.$$

Finally, we conclude that

$$(P(\bar{u}_h^{n+1}), \bar{u}_h^{n+1})_X \geq \frac{1}{2} (\|\bar{u}_h^{n+1}\|_X^2 - \|\bar{u}_h^n\|_X^2) - C \|\bar{u}_h^{n+1}\|_X.$$

Note that since $\|\bar{u}_h^n\|_X^2$ is given here, the right-hand side of this inequality is a second order polynomial function of $\|\bar{u}_h^{n+1}\|_X$ with positive leading order, thus there exists $k > 0$ such that if $\|\bar{u}_h^{n+1}\|_X \geq k$ then $(P(\bar{u}_h^{n+1}), \bar{u}_h^{n+1})_X > 0$. This implies that there exists \bar{u}_h^{n+1} such that $P(\bar{u}_h^{n+1}) = 0$, which proves Lemma 2. \square

Lemma 4. *If $(s_D^n, b_D^n, m_D^n, g_D^n)$ defined in (5) belongs to \mathcal{A} for all $D \in \mathcal{D}_h$, then any solution of the truncated system is physically admissible: $(s_D^{n+1}, b_D^{n+1}, m_D^{n+1}, g_D^{n+1}) \in \mathcal{A}$ for all $D \in \mathcal{D}_h$.*

Proof. We consider $(s_D^n, b_D^n, m_D^n, g_D^n)_{D \in \mathcal{D}_h} \in \mathcal{A}$, and let $\bar{u}_h^{n+1} \in X(\mathcal{D}_h)$ be a solution of the truncated discrete problem (32)–(35) as proved in Lemma 2.

Let $D \in \mathcal{D}_h$ such that $s_D^{n+1} = \min_{E \in \mathcal{D}_h} s_E^{n+1}$. We multiply equation (32) associated to D by $-(s_D^{n+1})^- = -\max(0, -s_D^{n+1}) \leq 0$:

$$\begin{aligned} -|D| (s_D^{n+1} - s_D^n) (s_D^{n+1})^- &= -\Delta t \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) (s_D^{n+1})^- \\ &\quad + \Delta t \sum_{E \in \mathcal{N}(D)} \tilde{F} \left(s_D^{n+1}, s_E^{n+1}, \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right) (s_D^{n+1})^- \\ &\quad - \Delta t |D| (K_1(m_D^n) \tilde{s}_D^{n+1} (1 - s_D^n) - H(g_D^n) \tilde{s}_D^{n+1}) (s_D^{n+1})^-. \end{aligned}$$

Using the monotony of the corrected operator, and the fact that $s_D^{n+1} \leq s_E^{n+1}$ for all $E \in \mathcal{D}_h$, we have

$$\mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) (s_D^{n+1})^- \geq 0.$$

Then using the properties of monotonicity and consistency \tilde{F} , it yields:

$$\begin{aligned} &\tilde{F} \left(s_D^{n+1}, s_E^{n+1}, \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right) (s_D^{n+1})^- \\ &\leq \tilde{F} \left(s_D^{n+1}, s_D^{n+1}, \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \right) (s_D^{n+1})^- \\ &= \tilde{V}_{D,E}^{n+1} (\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1}) \tilde{\chi} (s_D^{n+1}) (s_D^{n+1})^- = 0, \end{aligned}$$

since $\tilde{\chi} (s_D^{n+1}) = 0$ if $s_D^{n+1} \leq 0$ and $(s_D^{n+1})^- = 0$ otherwise.

Furthermore, we have

$$(K_1(m_D^n) \tilde{s}_D^{n+1} (1 - s_D^n) - H(g_D^n) \tilde{s}_D^{n+1}) (s_D^{n+1})^- = 0,$$

since $(s_D^{n+1})^- = 0$ if $s_D^{n+1} \geq 0$ and $\tilde{s}_D^{n+1} = 0$ otherwise.

Finally, we obtain

$$0 \leq (s_D^{n+1} - s_D^n) (s_D^{n+1})^- \leq s_D^{n+1} (s_D^{n+1})^- = -\left| (s_D^{n+1})^- \right|^2,$$

and then $s_D^{n+1} \geq 0$.

Similarly, we obtain $s_D^{n+1} \leq 1$, considering a control volume $D \in \mathcal{D}_h$ such that $s_D^{n+1} = \max_{E \in \mathcal{D}_h} s_E^{n+1}$

and multiplying equation (32) associated to D by $(s_D^{n+1} - 1)^+ = \max(0, s_D^{n+1} - 1)$. This proves that $0 \leq s_D^{n+1} \leq 1$ for all $D \in \mathcal{D}_h$. With similar arguments, we can establish the expected bounds on b_D^{n+1} , m_D^{n+1} and g_D^{n+1} , which proves Lemma 4. \square

Proposition 1 (Existence of an admissible solution). *If $(s_D^0, b_D^0, m_D^0, g_D^0) \in \mathcal{A}$ for all $D \in \mathcal{D}_h$, then the discrete problem (28)–(31) has a solution $(s_D^n, b_D^n, m_D^n, g_D^n)_{D \in \mathcal{D}_h}$ for all $n \in \mathbb{N}$, which is physically admissible:*

$$\forall n \in \mathbb{N}, \quad \forall D \in \mathcal{D}_h, \quad (s_D^n, b_D^n, m_D^n, g_D^n) \in \mathcal{A}.$$

Proof. We proceed by induction on $n \in \mathbb{N}$. The result is clear at $n = 0$ by assumption on the given initial data. If we assume that the admissible solution exists up to $n \in \mathbb{N}$, then there exists a physically admissible solution of the truncated discrete system (by Lemmas 2 and 4). But since it is physically admissible, then $\tilde{v}_D^{n+1} = v_D^{n+1}$, $v = s, b, m, g$, for all $D \in \mathcal{D}_h$, and then $\tilde{V}_{D,E}^{n+1} = V_{D,E}^{n+1}$ and $\tilde{F}(s_D^{n+1}, s_E^{n+1}, \tilde{V}_{D,E}^{n+1}(\tilde{m}_E^{n+1} - \tilde{m}_D^{n+1})) = F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1}(m_E^{n+1} - m_D^{n+1}))$, and finally $(s_D^{n+1}, b_D^{n+1}, m_D^{n+1}, g_D^{n+1})_{D \in \mathcal{D}_h}$ is an admissible solution of the original scheme. \square

4.3 Discrete a priori estimates

Proposition 2 (Discrete energy estimates). *Assume that $\Delta t_0 < \frac{1}{c_2}$, where the constant $c_2 > 0$ does not depend on the discretization parameters.*

Then for all $T > 0$ and all $\Delta t \leq \Delta t_0$, we have the following estimates: for all $N \in \mathbb{N}$ such that $N\Delta t \leq T$,

$$\sum_{n=0}^{N-1} \Delta t (\|s_h^{n+1}\|_{X_h}^2 + \|b_h^{n+1}\|_{X_h}^2 + \|m_h^{n+1}\|_{X_h}^2 + \|g_h^{n+1}\|_{X_h}^2) \leq \mathcal{C}, \quad (37)$$

where the constant \mathcal{C} does not depend on the discretization parameters.

Note that the condition on Δt_0 is not a CFL stability condition, since $c_2 > 0$ is independent of the space step discretization. It depends only on the physical parameters and it is not restrictive in practice.

Proof. To prove these a priori estimates, we adapt the proof of [9, Theorem 7] to our monotone combined scheme. Throughout this proof, C_i denotes constants which depend only on $f, V, \mathbf{D}, \Lambda, \Omega$ and $k_{\mathcal{T}}$, and not on the discretization parameters. We split the proof into several steps.

Step 1. We multiply the discrete equation of stem cells (28) by s_D^{n+1} and we sum over $D \in \mathcal{D}_h$. We get

$$E_{s,1} + E_{s,2} + E_{s,3} = \Delta t \sum_{D \in \mathcal{D}_h} |D| (K_1(m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1}) s_D^{n+1}, \quad (38)$$

where

$$\begin{aligned} E_{s,1} &= \sum_{D \in \mathcal{D}_h} |D| (s_D^{n+1} - s_D^n) s_D^{n+1} \geq \frac{1}{2} \sum_{D \in \mathcal{D}_h} |D| (|s_D^{n+1}|^2 - |s_D^n|^2), \\ E_{s,2} &= -\Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) s_D^{n+1}, \\ E_{s,3} &= \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1})) s_D^{n+1}. \end{aligned}$$

We treat the second term using the coercivity of the discrete corrected operator $\mathbb{S}^{\mathcal{D}_h}$ (22)

$$E_{s,2} \geq \Delta t C_S \|s_h^{n+1}\|_{X_h}^2.$$

Concerning $E_{s,3}$, we first perform a discrete integration by parts using the conservativity of the numerical flux F :

$$E_{s,3} = \frac{1}{2} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1})) (s_D^{n+1} - s_E^{n+1}).$$

Then, since $F(a, b, c) \leq |c| c_0$, it yields

$$\begin{aligned} E_{s,3} &\leq C_1 \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^{n+1} - m_D^{n+1}| |s_E^{n+1} - s_D^{n+1}| \\ &\leq \frac{C_1 \theta_1}{2} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^{n+1} - m_D^{n+1}|^2 \\ &\quad + \frac{C_1}{2\theta_1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |s_E^{n+1} - s_D^{n+1}|^2, \end{aligned}$$

using the Cauchy-Schwarz and Young inequalities. Combining (7) and (14) to estimate the second term of the right-hand side, we get

$$E_{s,3} \leq \frac{C_1 \theta_1}{2} \Delta t |\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 + \frac{C_2}{2\theta_1} \Delta t \|s_h^{n+1}\|_{X_h}^2,$$

where

$$|\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 := \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^{n+1} - m_D^{n+1}|^2. \quad (39)$$

Finally, we use the continuity of K_1 , H and the L^∞ bounds on s_D^n , s_D^{n+1} , m_D^n , g_D^n to estimate the right-hand side of (38):

$$\Delta t \sum_{D \in \mathcal{D}_h} |D| (K_1(m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1}) s_D^{n+1} \leq \Delta t M_1 |\Omega|.$$

To conclude, we have obtained the following estimate:

$$\begin{aligned} &\frac{1}{2} (\|\overline{s}_h^{n+1}\|_{L^2}^2 - \|\overline{s}_h^n\|_{L^2}^2) + \Delta t \left(C_S - \frac{C_2}{2\theta_1} \right) \|s_h^{n+1}\|_{X_h}^2 \\ &\leq \Delta t \frac{C_1 \theta_1}{2} |\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 + \Delta t M_1 |\Omega|. \end{aligned} \quad (40)$$

Step 2. In the same way, we multiply the scheme on osteogenic growth factor (31) by g_D^{n+1} and we sum over $D \in \mathcal{D}_h$. We get:

$$E_{g,1} + E_{g,2} = \Delta t \sum_{D \in \mathcal{D}_h} |D| (P(g_D^n) b_D^n - \delta_2 g_D^{n+1}) g_D^{n+1} \leq \Delta t M_4 |\Omega|,$$

where

$$\begin{aligned} E_{g,1} &= \sum_{D \in \mathcal{D}_h} |D| (g_D^{n+1} - g_D^n) g_D^{n+1} \geq \frac{1}{2} \sum_{D \in \mathcal{D}_h} |D| ((g_D^{n+1})^2 - (g_D^n)^2) = \frac{1}{2} (\|\overline{g}_h^{n+1}\|_{L^2}^2 - \|\overline{g}_h^n\|_{L^2}^2), \\ E_{g,2} &= -\Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \mathbb{G}_{D,E}^{n+1} (g_E^{n+1} - g_D^{n+1}) g_D^{n+1} \geq \Delta t C_G \|g_h^{n+1}\|_{X_h}^2. \end{aligned}$$

We finally obtain

$$\frac{1}{2} (\|\overline{g}_h^{n+1}\|_{L^2}^2 - \|\overline{g}_h^n\|_{L^2}^2) + \Delta t C_G \|g_h^{n+1}\|_{X_h}^2 \leq \Delta t M_4 |\Omega|. \quad (41)$$

Step 3. In order to get some estimates on $|\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2$ appearing in (40), we use the discrete equation (30) on bone matrix m . For that, we multiply it by $-\frac{1}{|D|} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| (m_E^{n+1} - m_D^{n+1})$, we sum over $D \in \mathcal{D}_h$ and we perform a discrete integration by parts:

$$\begin{aligned} & \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| (m_E^{n+1} - m_D^{n+1}) [(m_E^{n+1} - m_E^n) - (m_D^{n+1} - m_D^n)] \\ &= \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| (m_E^{n+1} - m_D^{n+1}) (f_3(b_E^{n+1}, m_E^{n+1}) - f_3(b_D^{n+1}, m_D^{n+1})). \end{aligned}$$

Consider now the Lipschitz constant of f_3 in \mathcal{A} , denoted by L_3 , and using again $a(a-b) \geq \frac{1}{2}(a^2 - b^2)$, we get by using the notation (39) that

$$\begin{aligned} & \frac{1}{2} \left[|\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 - |\overline{m}_h^n|_{1,\mathcal{D}_h}^2 \right] \\ & \leq L_3 \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^{n+1} - m_D^{n+1}| \left[|m_E^{n+1} - m_D^{n+1}| + |b_E^{n+1} - b_D^{n+1}| \right] \\ & \leq \Delta t \frac{3L_3}{2} \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^{n+1} - m_D^{n+1}|^2 + \Delta t \frac{L_3}{2} \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |b_E^{n+1} - b_D^{n+1}|^2. \end{aligned}$$

Finally, we have obtained

$$\frac{1}{2} \left[|\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 - |\overline{m}_h^n|_{1,\mathcal{D}_h}^2 \right] \leq \Delta t \frac{3L_3}{2} |\overline{m}_h^{n+1}|_{1,\mathcal{D}_h}^2 + \Delta t \frac{L_3}{2} |\overline{b}_h^{n+1}|_{1,\mathcal{D}_h}^2. \quad (42)$$

Step 4. Now we need to get some estimates on $|\overline{b}_h^{n+1}|_{1,\mathcal{D}_h}^2$. To this end, we multiply (33) by $-\frac{1}{|D|} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| (b_E^{n+1} - b_D^{n+1})$ and we sum over $D \in \mathcal{D}_h$. Following the same computations as in the previous step, we have for some $\theta_2 > 0$

$$\begin{aligned} & \frac{1}{2} \left[|\overline{b}_h^{n+1}|_{1,\mathcal{D}_h}^2 - |\overline{b}_h^n|_{1,\mathcal{D}_h}^2 \right] \leq \Delta t L_2 \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |b_E^{n+1} - b_D^{n+1}| \\ & \quad \times (|s_E^{n+1} - s_D^{n+1}| + |b_E^{n+1} - b_D^{n+1}| + |m_E^n - m_D^n| + |g_E^n - g_D^n|) \\ & \leq \Delta t L_2 \left(\frac{\theta_2}{2} + 2 \right) \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |b_E^{n+1} - b_D^{n+1}|^2 \\ & \quad + \frac{\Delta t L_2}{2\theta_2} \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |s_E^{n+1} - s_D^{n+1}|^2 \\ & + \frac{\Delta t L_2}{2} \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |m_E^n - m_D^n|^2 + \frac{\Delta t L_2}{2} \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |g_E^n - g_D^n|^2 \end{aligned}$$

Using again (7) and (14), we get:

$$\sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| |s_E^{n+1} - s_D^{n+1}|^2 \leq \frac{c_D(d+1)}{2dk_{\mathcal{T}}^2(d-1)^2} \|s_h^{n+1}\|_{X_h}^2.$$

We finally obtain:

$$\begin{aligned} \frac{1}{2} \left(\left| \bar{b}_h^{n+1} \right|_{1, \mathcal{D}_h}^2 - \left| \bar{b}_h^n \right|_{1, \mathcal{D}_h}^2 \right) &\leq \Delta t L_2 \left(\frac{\theta_2}{2} + 2 \right) \left| \bar{b}_h^{n+1} \right|_{1, \mathcal{D}_h}^2 + \Delta t \frac{C_3}{2\theta_2} \|s_h^{n+1}\|_{X_h}^2 \\ &\quad + \frac{\Delta t L_2}{2} |\bar{m}_h^n|_{1, \mathcal{D}_h}^2 + \frac{\Delta t L_2}{2} |\bar{g}_h^n|_{1, \mathcal{D}_h}^2. \end{aligned} \quad (43)$$

Step 5. Now we add the estimates (40)–(43):

$$\begin{aligned} &\frac{1}{2} (\|\bar{s}_h^{n+1}\|_{L^2}^2 - \|\bar{s}_h^n\|_{L^2}^2) + \frac{1}{2} (\|\bar{g}_h^{n+1}\|_{L^2}^2 - \|\bar{g}_h^n\|_{L^2}^2) \\ &+ \frac{1}{2} (|\bar{m}_h^{n+1}|_{1, \mathcal{D}_h}^2 - |\bar{m}_h^n|_{1, \mathcal{D}_h}^2) + \frac{1}{2} (|\bar{b}_h^{n+1}|_{1, \mathcal{D}_h}^2 - |\bar{b}_h^n|_{1, \mathcal{D}_h}^2) \\ &+ \Delta t \left(C_S - \frac{C_2}{2\theta_1} - \frac{C_3}{2\theta_2} \right) \|s_h^{n+1}\|_{X_h}^2 + \Delta t C_G \|g_h^{n+1}\|_{X_h}^2 \\ &\leq \Delta t (M_1 + M_4) |\Omega| + \Delta t \left(\frac{C_1 \theta_1}{2} + \frac{3 L_3}{2} \right) |\bar{m}_h^{n+1}|_{1, \mathcal{D}_h}^2 \\ &+ \Delta t \left(\frac{L_3}{2} + L_2 \left(\frac{\theta_2}{2} + 2 \right) \right) |\bar{b}_h^{n+1}|_{1, \mathcal{D}_h}^2 + \frac{\Delta t L_2}{2} |\bar{m}_h^n|_{1, \mathcal{D}_h}^2 + \frac{\Delta t L_2}{2} |\bar{g}_h^n|_{1, \mathcal{D}_h}^2. \end{aligned}$$

We choose θ_1 and θ_2 such that $C_S - \frac{C_2}{2\theta_1} - \frac{C_3}{2\theta_2} = \frac{C_S}{2}$ and we define

$$\begin{aligned} c_1 &= \max(2(M_1 + M_4)|\Omega|, L_2), \\ c_2 &= \max(C_1 \theta_1 + 3 L_3, L_3 + L_2(\theta_2 + 4)). \end{aligned}$$

We then derive the following energy estimate:

$$\begin{aligned} &\left(\|\bar{s}_h^{n+1}\|_{L^2}^2 + \|\bar{g}_h^{n+1}\|_{L^2}^2 + |\bar{b}_h^{n+1}|_{1, \mathcal{D}_h}^2 + |\bar{m}_h^{n+1}|_{1, \mathcal{D}_h}^2 \right) - \left(\|\bar{s}_h^n\|_{L^2}^2 + \|\bar{g}_h^n\|_{L^2}^2 + |\bar{b}_h^n|_{1, \mathcal{D}_h}^2 + |\bar{m}_h^n|_{1, \mathcal{D}_h}^2 \right) \\ &\quad + \Delta t C_S \|s_h^{n+1}\|_{X_h}^2 + 2 \Delta t C_G \|g_h^{n+1}\|_{X_h}^2 \\ &\leq c_1 \Delta t + c_2 \Delta t \left(|\bar{b}_h^{n+1}|_{1, \mathcal{D}_h}^2 + |\bar{m}_h^{n+1}|_{1, \mathcal{D}_h}^2 \right) + c_1 \Delta t (|\bar{m}_h^n|_{1, \mathcal{D}_h}^2 + |\bar{g}_h^n|_{1, \mathcal{D}_h}^2). \end{aligned} \quad (44)$$

It implies in particular that

$$y^{n+1} - y^n \leq c_1 \Delta t + c_1 \Delta t y^n + c_2 \Delta t y^{n+1},$$

with

$$y^n = \|\bar{s}_h^n\|_{L^2}^2 + \|\bar{g}_h^n\|_{L^2}^2 + |\bar{b}_h^n|_{1, \mathcal{D}_h}^2 + |\bar{m}_h^n|_{1, \mathcal{D}_h}^2.$$

Then we apply the Gronwall's lemma 8 proved in Appendix to get

$$\forall n \in \mathbb{N}, \quad n \Delta t \leq T \Rightarrow y^n \leq \left(y^0 + \frac{c_1}{c_1 + c_2} \right) \exp \left(\frac{(c_1 + c_2)T}{1 - c_2 \Delta t_0} \right),$$

with $\Delta t_0 < \frac{1}{c_2}$. We sum this inequality for $n = 0, \dots, N$ and get that:

$$\sum_{n=0}^N \Delta t y^n \leq (N+1) \Delta t \left(y^0 + \frac{c_1}{c_1 + c_2} \right) \exp \left(\frac{(c_1 + c_2)T}{1 - c_2 \Delta t_0} \right) \leq C_4,$$

which proves in particular

$$\sum_{n=0}^N \Delta t \left(|\bar{b}_h^n|_{1, \mathcal{D}_h}^2 + |\bar{m}_h^n|_{1, \mathcal{D}_h}^2 \right) \leq C_4.$$

Summing (44) over $n = 0, \dots, N-1$, we also obtain

$$\begin{aligned} y^N - y^0 + C_S \sum_{n=0}^{N-1} \Delta t \|s_h^{n+1}\|_{X_h}^2 + 2C_G \sum_{n=0}^{N-1} \Delta t \|g_h^{n+1}\|_{X_h}^2 \\ \leq c_1 T + c_2 \sum_{n=0}^{N-1} \Delta t y^{n+1} + c_1 \sum_{n=0}^{N-1} \Delta t y^n \\ \leq c_1 T + (c_1 + c_2) \sum_{n=0}^N \Delta t y^n \leq c_1 T + (c_1 + c_2) C_4, \end{aligned}$$

and thus

$$\sum_{n=0}^{N-1} \Delta t \left(\|s_h^{n+1}\|_{X_h}^2 + \|g_h^{n+1}\|_{X_h}^2 \right) \leq C_5.$$

We conclude using the fact that for $v = b, m$,

$$\begin{aligned} |\bar{v}_h|_{1, \mathcal{D}_h}^2 &= \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |\mathcal{D}_{D,E}| (v_E - v_D)^2 \geq \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \mathcal{D}_{D,E} (v_E - v_D)^2 \\ &= - \sum_{D \in \mathcal{D}_h} v_D \sum_{E \in \mathcal{N}(D)} \mathcal{D}_{D,E} (v_E - v_D) \geq C_D \|v_h\|_{X_h}^2. \end{aligned}$$

□

5 Convergence

5.1 Compactness of the approximate solution

To prove the compactity of the sequence \bar{u}_Δ , we need to bound the space and time translates of \bar{u}_Δ in order to use the Riesz-Fréchet-Kolmogorov theorem.

Lemma 5 (Space translates). *Assume $u_0 \in (H^1(\Omega))^4$. For any $\eta \in \mathbb{R}^d$, let $\Omega_\eta := \{x \in \Omega, x + \theta \eta \in \Omega, \forall \theta \in [0, 1]\}$. Then for all $T > 0$, for all $\Delta t \leq \Delta t_0 < \frac{1}{c_2}$, for all $\eta \in \mathbb{R}^d$, we have*

$$\int_0^T \int_{\Omega_\eta} |\bar{v}_\Delta(t, x + \eta) - \bar{v}_\Delta(t, x)|^2 dx dt \leq C^* |\eta| (|\eta| + \Delta), \quad \text{for } v_\Delta = s_\Delta, b_\Delta, m_\Delta, g_\Delta, \quad (45)$$

where C^* does not depend on the discretization parameters.

Proof. We follow the same guidelines as in [12, Lemma 9.2]. Let $\eta \in \mathbb{R}^d$, $\eta \neq 0$. We define for all $\sigma \in \mathcal{F}_h^{int}$

$$\chi_\sigma = \begin{cases} 1 & \text{if } [x, x + \eta] \cap \sigma \neq \emptyset, \\ 0 & \text{otherwise.} \end{cases}$$

A simple geometrical consideration leads to

$$|\bar{v}_\Delta(t, x + \eta) - \bar{v}_\Delta(t, x)| \leq \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} |v_E^{n+1} - v_D^{n+1}| \chi_{\sigma_{D,E}}(x) \text{ a.e. } x \in \Omega, \forall t \in (t^n, t^{n+1}].$$

Applying the Cauchy-Schwarz inequality, it yields

$$\begin{aligned} (\bar{v}_\Delta(t, x + \eta) - \bar{v}_\Delta(t, x))^2 &\leq \left(\sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \chi_{\sigma_{D,E}}(x) \text{diam}(K_{D,E}) \right) \\ &\quad \times \left(\sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \chi_{\sigma_{D,E}}(x) \frac{(v_E^{n+1} - v_D^{n+1})^2}{\text{diam}(K_{D,E})} \right), \end{aligned}$$

and then using [21, Lemma 3.4] we obtain

$$(\bar{v}_\Delta(t, x + \eta) - \bar{v}_\Delta(t, x))^2 \leq C(|\eta| + \Delta) \left(\sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \chi_{\sigma_{D,E}}(x) \frac{(v_E^{n+1} - v_D^{n+1})^2}{\text{diam}(K_{D,E})} \right),$$

where $C > 0$ only depends on d and $k_{\mathcal{T}}$. By integrating over $[0, T] \times \Omega_\eta$, we finally get

$$\begin{aligned} &\int_0^T \int_{\Omega_\eta} (\bar{v}_\Delta(t, x + \eta) - \bar{v}_\Delta(t, x))^2 dx dt \\ &\leq C(|\eta| + \Delta) \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \frac{(v_E^{n+1} - v_D^{n+1})^2}{\text{diam}(K_{D,E})} \int_0^T \int_{\Omega_\eta} \chi_{\sigma_{D,E}}(x) dx dt \\ &\leq C(|\eta| + \Delta) |\eta| \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \frac{|\sigma_{D,E}|}{d_{D,E}} (V_E^{n+1} - V_D^{n+1})^2 \\ &\leq C(|\eta| + \Delta) |\eta| \frac{(d+1)}{2(d-1)k_{\mathcal{T}}} \sum_{n=0}^{N-1} \Delta t \|v_h^{n+1}\|_{X_h}^2 \\ &\leq \mathcal{C}^*(|\eta| + \Delta) |\eta|, \end{aligned}$$

using $\int_{\Omega_\eta} \chi_{\sigma_{D,E}}(x) dx \leq |\eta| |\sigma_{D,E}|$, and estimates (8) and (37). \square

Lemma 6 (Time translates). *Assume $u_0 \in (H^1(\Omega))^4$. Let $T > 0$ and $\Delta t \leq \Delta t_0 < \frac{1}{c_2}$. There exists $K^* > 0$ not depending on the discretization parameters such that for all $\tau \in (0, T)$,*

$$\int_0^{T-\tau} \int_{\Omega} (\bar{v}_\Delta(t + \tau, x) - \bar{v}_\Delta(t, x))^2 dx dt \leq K^* \tau, \quad \text{for } v_\Delta = s_\Delta, b_\Delta, m_\Delta, g_\Delta. \quad (46)$$

Proof. We prove the result only for $v = s$, since other species can be treated in the same way. We follow the same guidelines as in [12, Lemma 9.6]. Let $\tau \in (0, T)$ and $t \in (0, T - \tau)$. We can write

$$\begin{aligned} \int_0^{T-\tau} \int_{\Omega} (\bar{s}_\Delta(t + \tau, x) - \bar{s}_\Delta(t, x))^2 dx dt &= \int_0^{T-\tau} \sum_{D \in \mathcal{D}_h} |D| \left(s_D^{n_1(t)} - s_D^{n_0(t)} \right)^2 dt, \\ &= \int_0^{T-\tau} \sum_{D \in \mathcal{D}_h} \left(s_D^{n_1(t)} - s_D^{n_0(t)} \right) \sum_{t \leq n \Delta t \leq t + \tau} |D| (s_D^{n+1} - s_D^n) dt, \end{aligned}$$

where $n_1(t) \in \{0, \dots, N-1\}$ is such that $t^{n_1} < t + \tau \leq t^{n_1} + 1$ and $n_0(t) \in \{0, \dots, N-1\}$ is such that $t^{n_0} < t \leq t^{n_0} + 1$.

Introducing

$$\chi(n, t) = \begin{cases} 1 & \text{if } t \leq (n+1)\Delta t < t + \tau \\ 0 & \text{otherwise} \end{cases},$$

and using the scheme (28), we get:

$$\int_0^{T-\tau} \int_{\Omega} (\bar{s}_{\Delta}(t + \tau, x) - \bar{s}_{\Delta}(t, x))^2 dx dt \leq B_1 + B_2 + B_3,$$

with

$$\begin{aligned} B_1 &:= \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \sum_{D \in \mathcal{D}_h} \left(s_D^{n_1(t)} - s_D^{n_0(t)} \right) \sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) dt, \\ B_2 &:= - \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \sum_{D \in \mathcal{D}_h} \left(s_D^{n_1(t)} - s_D^{n_0(t)} \right) \sum_{E \in \mathcal{N}(D)} F \left(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1}) \right) dt, \\ B_3 &:= \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \sum_{D \in \mathcal{D}_h} \left(s_D^{n_1(t)} - s_D^{n_0(t)} \right) |D| (K_1(m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1}) dt. \end{aligned}$$

Gathering by edges, we can write B_1 as

$$B_1 = \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \mathbb{S}_{D,E}^{n+1} (s_E^{n+1} - s_D^{n+1}) \left[\left(s_D^{n_1(t)} - s_E^{n_1(t)} \right) - \left(s_D^{n_0(t)} - s_E^{n_0(t)} \right) \right] dt.$$

Using (19) and (27), we have

$$\mathfrak{s}_{D,E} = \alpha \gamma_{D,E}(s_h) |S_D(s_h)| + \frac{|\sigma_{D,E}|}{d_{D,E}} = \alpha |\Lambda_{D,E}| + \frac{|\sigma_{D,E}|}{d_{D,E}},$$

and then

$$|\mathbb{S}_{D,E}^{n+1}| = |\Lambda_{D,E}^{n+1} + \mathfrak{s}_{D,E}^{n+1}| \leq (1 + \alpha) |\Lambda_{D,E}^{n+1}| + \frac{|\sigma_{D,E}|}{d_{D,E}}.$$

Using the continuity of Λ , the boundedness of m and (14), we obtain

$$|\mathbb{S}_{D,E}^{n+1}| \leq C |\mathcal{D}_{D,E}| + \frac{|\sigma_{D,E}|}{d_{D,E}} \leq C (\text{diam}(K_{D,E}))^{d-2} + \frac{|\sigma_{D,E}|}{d_{D,E}}, \quad (47)$$

where C is a constant independent of the discretization parameters. Using Cauchy-Schwarz and Young inequalities and the estimate (47), we obtain $B_1 \leq C(T_1 + T_2 + T_3)$, with

$$\begin{aligned} T_1 &= \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \|s_h^{n+1}\|_{X_h}^2 dt, \\ T_2 &= \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \|s_h^{n_1(t)}\|_{X_h}^2 dt, \\ T_3 &= \sum_{n=0}^{N-1} \Delta t \int_0^{T-\tau} \chi(n, t) \|s_h^{n_0(t)}\|_{X_h}^2 dt. \end{aligned}$$

Then using $\int_0^{T-\tau} \chi(n, t) dt \leq \tau$ and a priori estimate (37), we have that $T_1 \leq C \tau$. Then following [12, Lemma 9.6],

$$T_2 = \sum_{m=0}^{N-1} \int_{m\Delta t}^{(m+1)\Delta t} \Delta t \sum_{n=0}^{N-1} \chi(n, t) \|s_h^m\|_{X_h}^2 dt \leq C \tau,$$

and in the same way $T_3 \leq C \tau$, which yields $B_1 \leq C \tau$.

The terms B_2 and B_3 can be treated using the same kind of arguments, together with the properties of the flux function F and of the reaction terms. \square

We will deduce the convergence of u_Δ from that of \bar{u}_Δ using the following lemma, proved in [20, Lemma 1.5.4].

Lemma 7 (see [20]). *The sequence $(u_\Delta - \bar{u}_\Delta)_\Delta$ converges strongly to zero in $L^2(Q_T)$ as $\Delta \rightarrow 0$.*

Using estimates (45), (46) and applying the Riesz-Fréchet-Kolmogorov criterion of strong compactness [5, Theorem IV.25], $(\bar{u}_\Delta)_\Delta$ is relatively compact in $(L^2(Q_T))^4$, and then there exists a subsequence still denoted $(\bar{u}_\Delta)_\Delta$ which converges strongly to some function $u \in (L^2(Q_T))^4$. Thus due to Lemma 7, $(u_\Delta)_\Delta$ converges strongly to $u \in (L^2(Q_T))^4$. Moreover, due to the space translate estimate (45), we obtain that $u \in (L^2(0, T; H^1(\Omega)))^4$ (see for example [11, Theorem 1]). Finally, we have established the following result:

Proposition 3 (Strong convergence in $L^2(Q_T)$). *There exists $u \in (L^2(0, T; H^1(\Omega)))^4$ and a subsequence of $(u_\Delta)_\Delta$, still denoted $(u_\Delta)_\Delta$, such that*

$$u_\Delta \rightarrow u \text{ in } (L^2(Q_T))^4 \text{ strongly, as } \Delta \rightarrow 0.$$

5.2 Convergence of the scheme

We now prove that the limit u given in Proposition 3 is a weak solution to the continuous problem.

Theorem 1 (Convergence of the scheme (28)–(31)). *The limit u defined in Proposition 3 is a weak admissible solution (in the sense of Definition 1) of the problem (1)–(4).*

Proof. Let us focus our convergence analysis on the stem cells equation. Other species can be treated in the same way.

Let $\psi \in \mathcal{D}([0, T) \times \bar{\Omega})$ and define the sequence $(\psi_D^n)_{D \in \mathcal{D}_h, n \in \{0, \dots, N\}}$ by $\psi_D^n = \psi(t^n, P_D)$. Multiplying equation (28) by ψ_D^{n+1} and summing over $D \in \mathcal{D}_h, n \in \{0, \dots, N-1\}$, we get:

$$A_\Delta + B_\Delta + C_\Delta = F_\Delta,$$

where

$$\begin{aligned}
A_\Delta &= \sum_{n=0}^{N-1} \sum_{D \in \mathcal{D}_h} |D| (s_D^{n+1} - s_D^n) \psi_D^{n+1}, \\
B_\Delta &= - \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \mathbb{S}_{D,E}^{n+1} s_E^{n+1} \psi_D^{n+1}, \\
C_\Delta &= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} F \left(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1}) \right) \psi_D^{n+1}, \\
F_\Delta &= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} |D| \left(K_1 (m_D^n) s_D^{n+1} (1 - s_D^n) - H(g_D^n) s_D^{n+1} \right) \psi_D^{n+1}.
\end{aligned}$$

Time evolution term. Integrating by parts with respect to time the first term and using the strong convergence of $(s_\Delta)_\Delta$, we obtain classically that:

$$A_\Delta \longrightarrow - \int_{Q_T} s \partial_t \psi \, dx \, dt - \int_{\Omega} s_0(x) \psi(0, x) \, dx \quad \text{as } \Delta \rightarrow 0.$$

Diffusion term. Using the definition of the corrected diffusive operator, we have

$$B_\Delta = B_\Delta^1 + B_\Delta^2,$$

with

$$\begin{aligned}
B_\Delta^1 &= - \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \Lambda_{D,E}^{n+1} s_E^{n+1} \psi_D^{n+1}, \\
B_\Delta^2 &= - \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \mathfrak{s}_{D,E}^{n+1} s_E^{n+1} \psi_D^{n+1}.
\end{aligned}$$

To deal with B_Δ^1 , we use the definition (13) of $\Lambda_{D,E}^{n+1}$ and denoting

$$\tilde{\Lambda}_\Delta|_{(t^n, t^{n+1}] \times K} := \Lambda_K^{n+1},$$

we get:

$$\begin{aligned}
B_\Delta^1 &= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} \sum_{K \in \mathcal{T}_h} \Lambda_K^{n+1} \left(\int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D \, dx \right) s_E^{n+1} \psi_D^{n+1} \\
&= \sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{T}_h} \int_K \tilde{\Lambda}_h^{n+1} \mathbf{D}(x) \nabla s_h^{n+1}(x) \cdot \nabla \left(\sum_{D \in \mathcal{D}_h} \psi_D^{n+1} \varphi_D(x) \right) dx \\
&= B_\Delta^{1,1} + B_\Delta^{1,2},
\end{aligned}$$

with

$$\begin{aligned}
B_\Delta^{1,1} &= \sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{T}_h} \int_K \tilde{\Lambda}_h^{n+1} \mathbf{D}(x) \nabla s_h^{n+1}(x) \cdot \nabla (I_\psi(t^{n+1}, x) - \psi(t^{n+1}, x)) \, dx, \\
B_\Delta^{1,2} &= \sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{T}_h} \int_K \tilde{\Lambda}_h^{n+1} \mathbf{D}(x) \nabla s_h^{n+1}(x) \cdot \nabla \psi(t^{n+1}, x) \, dx,
\end{aligned}$$

where

$$I_\psi(t^{n+1}, x) = \sum_{D \in \mathcal{D}_h} \psi_D^{n+1} \varphi_D(x).$$

It is proved in [14, Section 6.2.2] that $B_\Delta^{1,1} \rightarrow 0$ as $\Delta \rightarrow 0$. It remains to prove that

$$B_\Delta^{1,2} \longrightarrow \int_{Q_T} \mathbf{D}(x) \Lambda(m) \nabla s \cdot \nabla \psi \, dx \, dt \quad \text{as } \Delta \rightarrow 0.$$

To this end, we write

$$B_\Delta^{1,2} - \int_{Q_T} \mathbf{D}(x) \Lambda(m) \nabla s \cdot \nabla \psi \, dx \, dt = B_\Delta^{1,2,1} + B_\Delta^{1,2,2},$$

with

$$\begin{aligned} B_\Delta^{1,2,1} &= \sum_{n=0}^{N-1} \int_{t^n}^{t^{n+1}} \sum_{K \in \mathcal{T}_h} \int_K \mathbf{D}(x) \tilde{\Lambda}_h^{n+1}(x) \nabla s_h^{n+1}(x) \cdot \nabla (\psi(t^{n+1}, x) - \psi(t, x)) \, dx \, dt, \\ B_\Delta^{1,2,2} &= \int_{Q_T} \mathbf{D}(x) (\tilde{\Lambda}_\Delta \nabla s_\Delta - \Lambda(m) \nabla s) \cdot \nabla \psi \, dx \, dt. \end{aligned}$$

We now prove that $B_\Delta^{1,2,1}$ and $B_\Delta^{1,2,2}$ tend to zero as Δ tends to zero. Using the regularity of ψ , we have for $t \in (t^n, t^{n+1}]$:

$$|\nabla \psi(t^{n+1}, x) - \nabla \psi(t, x)| \leq C_\psi \Delta t,$$

and then using the L^∞ boundedness of \mathbf{D} and $\tilde{\Lambda}_h^{n+1}$, we get

$$\begin{aligned} |B_\Delta^{1,2,1}| &\leq \Delta t C \sum_{n=0}^{N-1} \Delta t \|s_h^{n+1}\|_{X_h} |\Omega|^{\frac{1}{2}} \leq \Delta t C T^{\frac{1}{2}} |\Omega|^{\frac{1}{2}} \left(\sum_{n=0}^{N-1} \Delta t \|s_h^{n+1}\|_{X_h}^2 \right)^{\frac{1}{2}} \\ &\leq C \Delta t \longrightarrow 0 \quad \text{as } \Delta \rightarrow 0. \end{aligned}$$

To treat the term $B_\Delta^{1,2,2}$, we use the fact that $\nabla s_\Delta \rightarrow \nabla s$ weakly in $(L^2(Q_T))^d$. This result can be established following the same proof as in [14, Section 6.2.2]. Moreover, using Lemma 9, the strong convergence of m_Δ to m in $L^2(Q_T)$ and the continuity of Λ , we have that:

$$\tilde{\Lambda}_\Delta \rightarrow \Lambda(m) \text{ strongly in } L^2(Q_T) \text{ as } \Delta \rightarrow 0.$$

Then using these two facts, the a priori estimate (37) and the boundedness of \mathbf{D} , $\nabla \psi$ and $\Lambda(m)$, it is clear that $B_\Delta^{1,2,2}$ tends to zero as $\Delta \rightarrow 0$.

It remains now to ensure that the corrective term B_Δ^2 tends to zero. We write:

$$|B_\Delta^2| \leq \frac{1}{2} \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \mathfrak{s}_{D,E}^{n+1} |s_D^{n+1} - s_E^{n+1}| |\psi_D^{n+1} - \psi_E^{n+1}|.$$

Since ψ is regular enough, there exists a positive constant C_ψ such that

$$|\psi_D^{n+1} - \psi_E^{n+1}| \leq 2 C_\psi \text{diam}(D).$$

Using this last inequality, according to assumption (P3) on the monotone correction, the corrective term vanishes.

Haptotaxis term. For each couple of control volumes $D, E \in \mathcal{D}_h$, we define

$$(V\chi)_{D,E}^{n+1} := - \sum_{K \in \mathcal{T}_h} V_K^{n+1} \chi(s_K^{n+1}) \int_K \mathbf{D}(x) \nabla \varphi_E \cdot \nabla \varphi_D dx.$$

We note that for $D \in \mathcal{D}_h$ and $E \in \mathcal{N}(D)$ (then $E \neq D$), $(V\chi)_{D,E}^{n+1} = V_{D,E}^{n+1} \chi(s_{K_{D,E}}^{n+1})$, with $V_{D,E}^{n+1}$ defined by (13) and $s_{K_{D,E}}$ defined by (16). We set

$$C_\Delta^* := \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} (V\chi)_{D,E}^{n+1} (m_E^{n+1} - m_D^{n+1}) \psi_D^{n+1}.$$

On the one hand, it is clear that

$$C_\Delta^* \rightarrow - \int_{Q_T} \mathbf{D}(x) V(m) \chi(s) \nabla m \cdot \nabla \psi dx dt \quad \text{as } \Delta \rightarrow 0.$$

Indeed, since $(V\chi)_{D,D} = - \sum_{E \in \mathcal{N}(D)} (V\chi)_{D,E}$, we write

$$\begin{aligned} C_\Delta^* &= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{D}_h} (V\chi)_{D,E}^{n+1} m_E^{n+1} \psi_D^{n+1} \\ &= - \sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{T}_h} \int_K \mathbf{D}(x) V_K^{n+1} \chi(s_K^{n+1}) \nabla m_h^{n+1} \cdot \nabla I_\psi(t^{n+1}, x) dx \\ &= - \sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{T}_h} \int_K \mathbf{D}(x) \tilde{V}_\Delta \chi(\tilde{s}_\Delta) \nabla m_\Delta \cdot \nabla I_\psi(t^{n+1}, x) dx \\ &\rightarrow - \int_{Q_T} \mathbf{D}(x) V(m) \chi(s) \nabla m \cdot \nabla \psi dx dt, \end{aligned}$$

using the strong convergence of \tilde{V}_Δ and $\chi(\tilde{s}_\Delta)$ to $V(m)$ and $\chi(s)$ respectively, and the weak convergence of ∇m_Δ to ∇m .

On the other hand, we have

$$\begin{aligned} C_\Delta - C_\Delta^* &= \frac{1}{2} \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \left(F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1}(m_E^{n+1} - m_D^{n+1})) - V_{D,E}^{n+1} \chi(s_{K_{D,E}}^{n+1})(m_E^{n+1} - m_D^{n+1}) \right) \\ &\quad \times (\psi_D^{n+1} - \psi_E^{n+1}). \end{aligned}$$

But using the consistency and the Lipschitz properties the numerical flux function F , we have:

$$\begin{aligned} &\left| F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1}(m_E^{n+1} - m_D^{n+1})) - V_{D,E}^{n+1} \chi(s_{K_{D,E}}^{n+1})(m_E^{n+1} - m_D^{n+1}) \right| \\ &= \left| F(s_D^{n+1}, s_E^{n+1}, V_{D,E}^{n+1}(m_E^{n+1} - m_D^{n+1})) - F(s_{K_{D,E}}^{n+1}, s_{K_{D,E}}^{n+1}, V_{D,E}^{n+1}(m_E^{n+1} - m_D^{n+1})) \right| \\ &\leq L_M \left| V_{D,E}^{n+1} \right| |m_E^{n+1} - m_D^{n+1}| \left(\left| s_D^{n+1} - s_{K_{D,E}}^{n+1} \right| + \left| s_E^{n+1} - s_{K_{D,E}}^{n+1} \right| \right). \end{aligned}$$

Then it yields

$$|C_\Delta - C_\Delta^*| \leq \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |V_{D,E}^{n+1}| |m_E^{n+1} - m_D^{n+1}| |s_D^{n+1} - s_{K_{D,E}}^{n+1}| |\psi_D^{n+1} - \psi_E^{n+1}|.$$

Since $|V_{D,E}^{n+1}| \leq C |\mathcal{D}_{D,E}| \leq C \text{diam}(K_{D,E})^{d-2}$ and $|\psi_D^{n+1} - \psi_E^{n+1}| \leq C \text{diam}(K_{D,E})$, we get using the Cauchy-Schwarz inequality:

$$\begin{aligned} |C_\Delta - C_\Delta^*| &\leq C \left(\sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \frac{\text{diam}(K_{D,E})^{2(d-1)}}{|D \cap K_{D,E}|} |m_E^{n+1} - m_D^{n+1}|^2 \right)^{1/2} \\ &\quad \times \left(\sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} |D \cap K_{D,E}| |s_D^{n+1} - s_{K_{D,E}}^{n+1}|^2 \right)^{1/2}. \end{aligned}$$

But following from geometrical properties of a simplex K , we have

$$\frac{\text{diam}(K_{D,E})^{2(d-1)}}{|D \cap K_{D,E}|} \leq C \frac{|K_{D,E}|}{|D \cap K_{D,E}|} \text{diam}(K_{D,E})^{d-1} \leq C \text{diam}(K_{D,E})^{d-1} \leq C h \text{diam}(K_{D,E})^{d-2},$$

which yields

$$|C_\Delta - C_\Delta^*| \leq C \sqrt{h} \left(\sum_{n=0}^{N-1} \Delta t \|m_h^{n+1}\|_{X_h}^2 \right)^{1/2} \|\bar{s}_\Delta - \tilde{s}_\Delta\|_{L^2} \rightarrow 0 \text{ as } \Delta \rightarrow 0,$$

using Lemma 9 proved in Appendix.

Source term. The strong convergence of the sequence $(u_\Delta)_\Delta$ to u and the continuity of the function $(s_1, s_2, m, g) \mapsto K_1(m) s_2 (1 - s_1) - H(g) s_2$ yield:

$$F_\Delta \longrightarrow \int_{Q_T} f_1(s, m, g) \psi \, dx \, dt.$$

□

6 Numerical experiments

In this section, we present some numerical results which illustrates the efficiency of our corrected combined finite volume–finite element scheme. To implement the semi-implicit scheme (28)–(31), we use the Newton’s method coupled with a biconjugate gradient method to solve the nonlinear system. While the discrete maximum principle is not satisfied, the monotone correction is computed using the iterative algorithm described in [7]. In this article, the convergence rate of the corrected scheme is studied for a Poisson equation. It is shown that the rate of convergence is close to 1, which is a little less than that of the non corrected scheme, due to the artificial diffusion introduced by the monotone correction.

We simulate the healing of a long bone in rats [19]. The simulation corresponds to a 0.2 cm fracture. The geometry of the fracture is described on Figure 2. Initially, the domain contains only the bone (the black area corresponds to $m_0 = 1$), and two cell clusters along the broken bone consisting of stem cells and growth factor (the grey area corresponds to $s_0 = 1$ and $g_0 = 20$). Elsewhere there is nothing initially. The physical parameters are the following:

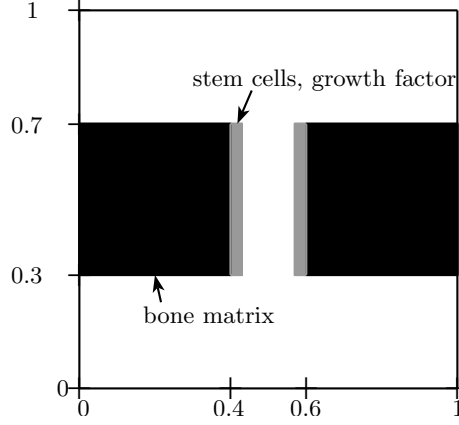


Figure 2: Geometry and initial condition.

	Min. Val. s	Max. Val. s	Min. Val. g	Max. Val. g
Iter. 1	9.47×10^{-21}	0.999	9.9×10^{-21}	19.8
Iter. 10	5.83×10^{-21}	0.991	9.05×10^{-21}	17.99

Table 1: Results obtained with the non corrected scheme on an admissible mesh.

Diffusion coefficient $\Lambda(m)$	$\chi_h = 0.004, \zeta_h = 0.025, \lambda_0 = 10^{-5}$
Diffusion coefficient Λ_g	$\Lambda_g = 0.005$
Haptotaxis velocity $V(m)$	$\chi_k = 0.0034, \zeta_k = 0.5$
Reaction term f_1	$\alpha_1 = 1.01, \beta_1 = 0.1, \gamma_1 = 10, \eta_1 = 1$
Reaction term f_2	$\alpha_2 = 0.202, \beta_2 = 0.1, \rho = 1, \delta_1 = 0.1$
Reaction term f_3	$\lambda = 2$
Reaction term f_4	$\delta_2 = 100, \gamma_2 = 1000, \eta_2 = 1$

Isotropic case. We first assume that $\mathbf{D} \equiv I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. We consider an admissible mesh made of 14336 triangles and 21632 edges. Especially, all the angles are acute which ensures in this case that the combined finite volume–finite element scheme without correction (9)–(12) satisfies the maximum principle. In particular, we observe in Table 1 that the discrete unknowns remain nonnegative.

Then we consider three general unstructured meshes containing obtuse angles:

	Mesh 1	Mesh 2	Mesh 3
Number of triangles	1539	3132	15568
Number of edges	2346	4756	23479

In Table 2, we present the minimum and maximum values of s and g obtained with the scheme without and with monotone correction, after 10 iterations. We clearly observe that the discrete maximum principle is well respected after correction, with disappearance of the undershoots.

		Mesh 1	Mesh 2	Mesh 3
Without correction after 10 it.	Undershoots s	16	16	92
	Min. Val. s	-2.67×10^{-4}	-8.95×10^{-7}	-3.01×10^{-4}
	Max. Val. s	0.990	0.991	0.992
	Undershoots g	70	71	144
	Min. Val. g	-0.27	-1.01×10^{-2}	-8.56×10^{-3}
	Max. Val. g	17.96	18.41	20.27
With correction after 10 it.	Min. Val. s	9.58×10^{-6}	1.18×10^{-6}	3.93×10^{-6}
	Max. Val. s	0.989	0.990	0.99
	Min. Val. g	1.51×10^{-4}	8.02×10^{-5}	7.68×10^{-5}
	Max. Val. g	17.81	18.33	19.37

Table 2: Numerical results obtained with the original scheme (9)–(12) and the corrected scheme (28)–(31) after 10 iterations.

Finally, we consider the monotone scheme (28)–(31) on the finest mesh 3. After two days, we observe the formation of osteoblasts (Figure 3(b)) where the stem cells were initially concentrated in presence of the growth factor g . These osteoblasts synthesized the new bone matrix (Figure 3(c)). The mineralization front is represented on Figure 4. The stem cells moved towards the center of the fracture (Figure 3(a)). These results are in agreement with previous results [9, 19].

Anisotropic rotating case. We now assume that $\mathbf{D} = \begin{pmatrix} 1.5 & 1 \\ 1 & 2 \end{pmatrix}$. Since \mathbf{D} is a positive-definite matrix, it is diagonalizable in an orthonormal basis, that is

$$\mathbf{D} = P \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} P^{-1},$$

where the eigenvalues are $\lambda_1 = 2.7808$, $\lambda_2 = 0.7192$, and P is the rotation matrix corresponding to an angle of approximately 0.89 radians.

We consider the monotone scheme (28)–(31) on the finest mesh 3, and observe its ability to take into account a full tensor. The results obtained after two days are represented on Figure 5. In spite of anisotropy, we still obtain physically admissible solutions. Moreover, we observe the effect of this choice of tensor \mathbf{D} corresponding to a rotation of 0.89 radians, which favors a slanting diffusion.

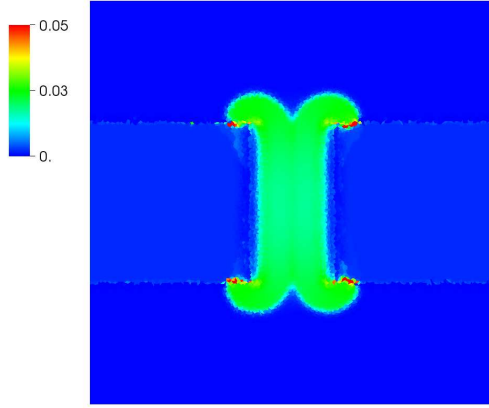
Appendix

Lemma 8 (Discrete Gronwall's inequality). *Given $c_1 > 0$ and $c_2 > 0$, assume that*

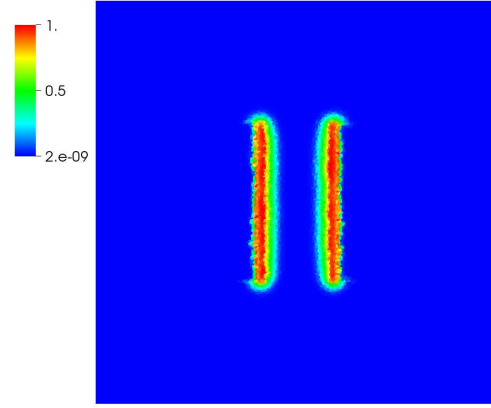
$$y^{n+1} - y^n \leq c_1 \Delta t + c_1 \Delta t y^n + c_2 \Delta t y^{n+1} \quad \forall n \in \mathbb{N}.$$

Given a fixed time step $\Delta t_0 < \frac{1}{c_2}$ and a fixed time $T > 0$, we have for all $\Delta t \leq \Delta t_0$:

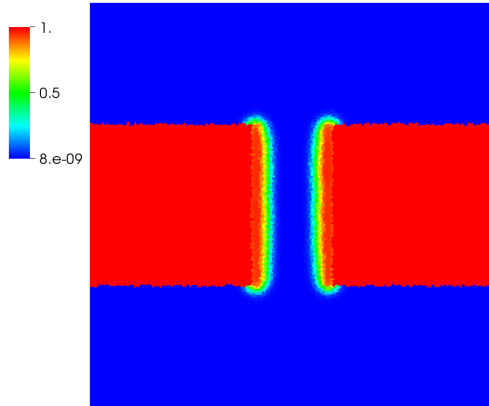
$$\forall n \in \mathbb{N}, \quad n \Delta t \leq T \Rightarrow y^n \leq \left(y^0 + \frac{c_1}{c_1 + c_2} \right) \exp \left(\frac{(c_1 + c_2)T}{1 - c_2 \Delta t_0} \right).$$



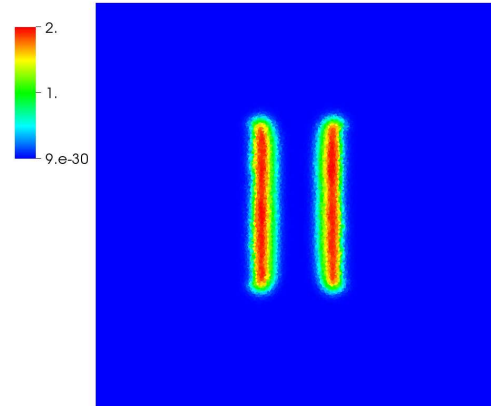
(a) Concentration of stem cells s



(b) Concentration of osteoblasts b



(c) Bone matrix density m



(d) Concentration of the growth factor g

Figure 3: Bone matrix density, concentrations of stem cells, osteoblasts and growth factor at $T = 2$ days in the isotropic case.

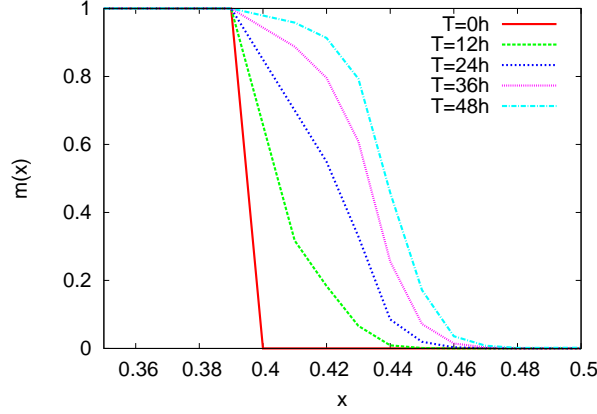


Figure 4: Bone matrix density along the line $y = 0.175$.

Proof. Since $\Delta t \leq \Delta t_0 < \frac{1}{c_2}$, we have

$$y^{n+1} \leq \left(\frac{1 + c_1 \Delta t}{1 - c_2 \Delta t} \right) y^n + \frac{c_1 \Delta t}{1 - c_2 \Delta t}.$$

Denoting $\alpha = \frac{1 + c_1 \Delta t}{1 - c_2 \Delta t} > 1$ and $\beta = \frac{1}{1 - c_2 \Delta t}$, we obtain by a straightforward recursion that

$$\forall n \in \mathbb{N}, \quad y^n \leq \alpha^n y^0 + \beta c_1 \Delta t \sum_{k=0}^{n-1} \alpha^k = \alpha^n y^0 + \beta c_1 \Delta t \frac{\alpha^n - 1}{\alpha - 1}.$$

Using that $\frac{\beta}{\alpha - 1} = \frac{1}{(c_1 + c_2)\Delta t}$ and $\alpha^n - 1 \leq \alpha^n$, it yields

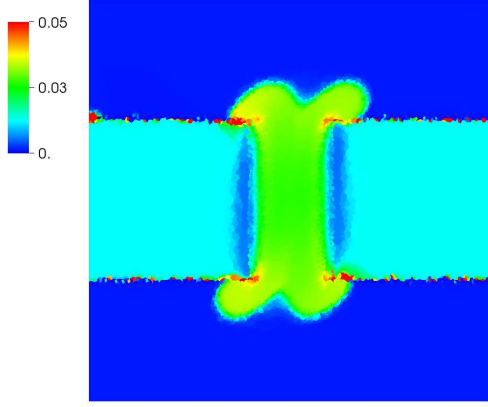
$$\forall n \in \mathbb{N}, \quad y^n \leq \left(y^0 + \frac{c_1}{c_1 + c_2} \right) \alpha^n.$$

Moreover, since $\alpha = 1 + \lambda \Delta t$ with $\lambda = \frac{c_1 + c_2}{1 - c_2 \Delta t}$, we have

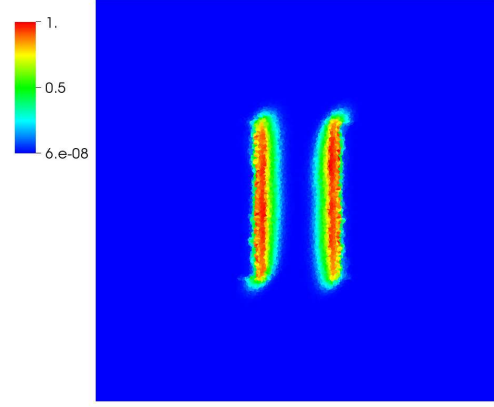
$$\alpha^n = (1 + \lambda \Delta t)^n \leq \exp(\lambda n \Delta t),$$

and finally, using that $\Delta t \leq \Delta t_0$, we obtain the result. \square

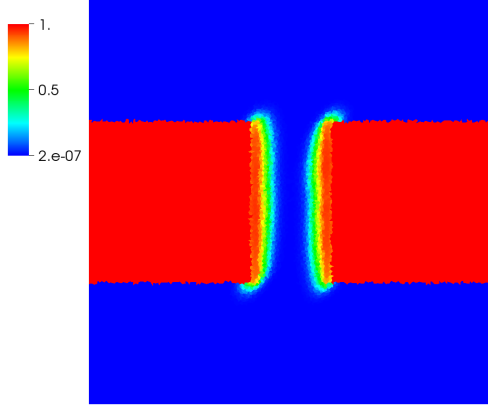
Lemma 9. Let $(u_D^{n+1})_{D \in \mathcal{D}_h, n \in \{0, \dots, N\}} \in \mathbb{R}^{\text{Card}(\mathcal{D}_h) \times (N+1)}$, \bar{u}_Δ the corresponding finite volume solution on \mathcal{D}_h and \tilde{u}_Δ the corresponding function piecewise constant on \mathcal{T}_h (see Definition 2). Then $(\bar{u}_\Delta - \tilde{u}_\Delta)_\Delta$ converges strongly to 0 in $L^2(Q_T)$ as Δ tends to 0.



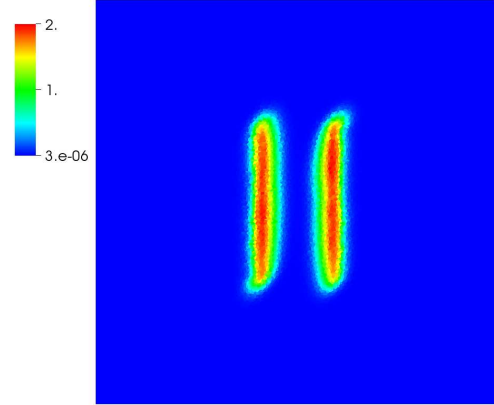
(a) Concentration of stem cells s



(b) Concentration of osteoblasts b



(c) Bone matrix density m



(d) Concentration of the growth factor g

Figure 5: Bone matrix density, concentrations of stem cells, osteoblasts and growth factor at $T = 2$ days in the anisotropic rotating case.

Proof. Using Definition 2, we have

$$\begin{aligned}
\int_{Q_T} |\bar{u}_\Delta - \tilde{u}_\Delta|^2 dx dt &= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{\substack{K \in \mathcal{T}_h \\ |K \cap D| \neq 0}} \int_{K \cap D} |u_D^{n+1} - u_K^{n+1}|^2 dx \\
&= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{\substack{K \in \mathcal{T}_h \\ |K \cap D| \neq 0}} |K \cap D| \left| u_D^{n+1} - \frac{1}{\text{Card}(\mathcal{D}_K)} \sum_{E \in \mathcal{D}_K} u_E^{n+1} \right|^2 \\
&= \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{\substack{K \in \mathcal{T}_h \\ |K \cap D| \neq 0}} \frac{|K \cap D|}{\text{Card}(\mathcal{D}_K)^2} \left| \sum_{E \in \mathcal{D}_K} (u_D^{n+1} - u_E^{n+1}) \right|^2 \\
&\leq \sum_{n=0}^{N-1} \Delta t \sum_{D \in \mathcal{D}_h} \sum_{\substack{K \in \mathcal{T}_h \\ |K \cap D| \neq 0}} \frac{|K \cap D|}{\text{Card}(\mathcal{D}_K)} \sum_{E \in \mathcal{D}_K} (u_D^{n+1} - u_E^{n+1})^2.
\end{aligned}$$

But since it holds

$$\sum_{D \in \mathcal{D}_h} \sum_{\substack{K \in \mathcal{T}_h \\ |K \cap D| \neq 0}} \sum_{E \in \mathcal{D}_K} (u_D - u_E) = \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} (u_D - u_E) = 2 \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} (u_D - u_E),$$

we finally get

$$\int_{Q_T} |\bar{u}_\Delta - \tilde{u}_\Delta|^2 dx dt \leq \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} |K_{D,E}| (u_D^{n+1} - u_E^{n+1})^2.$$

Then since $|K_{D,E}| \leq C (\text{diam}(K_{D,E}))^{d-1}$, we obtain

$$\begin{aligned}
\int_{Q_T} |\bar{u}_\Delta - \tilde{u}_\Delta|^2 dx dt &\leq C h \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{D,E} \in \mathcal{F}_h^{int}} \text{diam}(K_{D,E})^{d-2} (u_D^{n+1} - u_E^{n+1})^2 \\
&\leq C h \sum_{n=0}^{N-1} \Delta t \|u_h^{n+1}\|_{X_h}^2 \leq C h \rightarrow 0 \text{ as } \Delta \rightarrow 0.
\end{aligned}$$

□

Acknowledgements: M. B.-C. was partially supported by the ANR project GEONUM (ANR-12-IS01-0004-01) and by the ANR project ACHYLLES (ANR-14-CE25-0001-03).

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